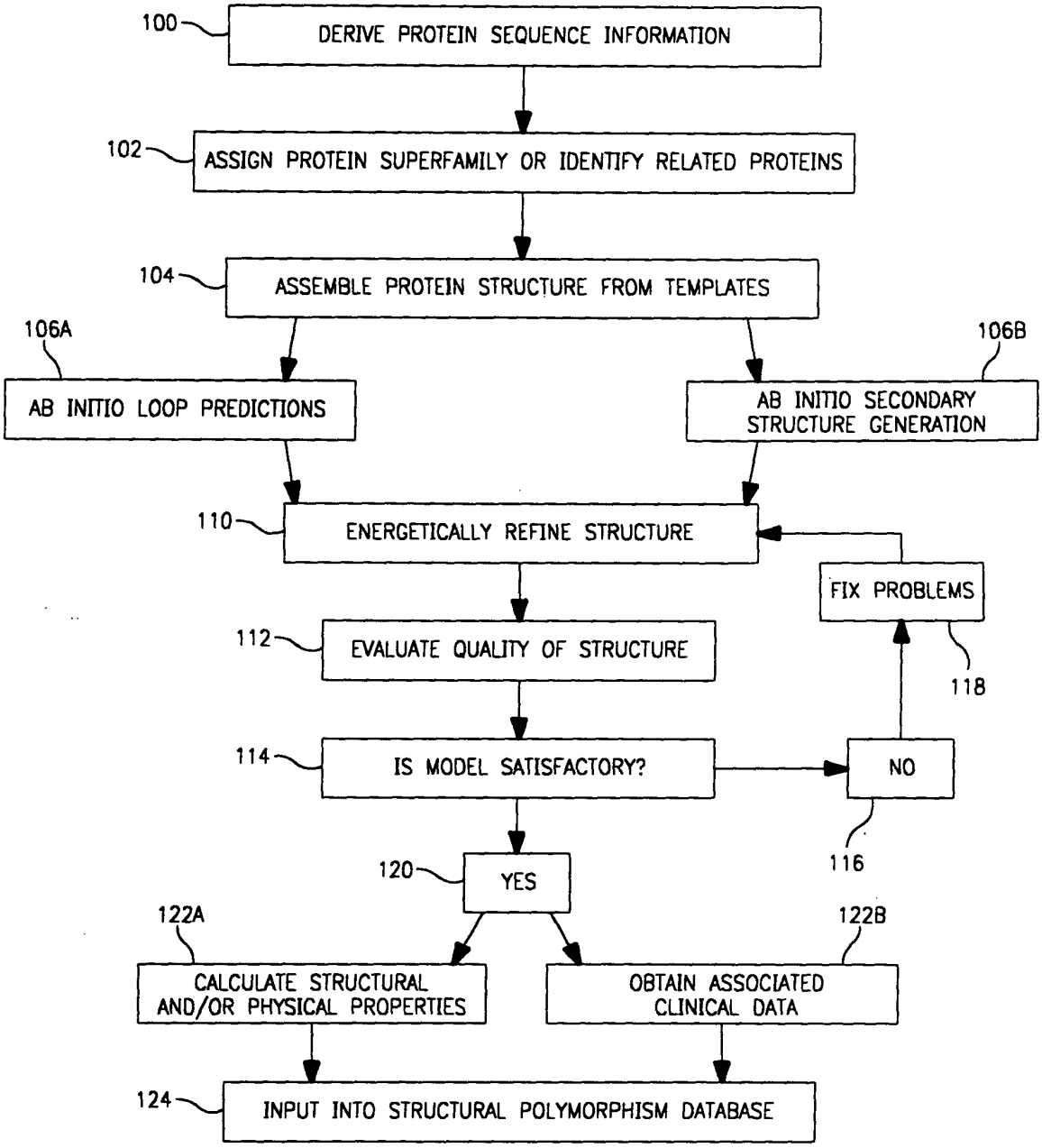



FIG. 1

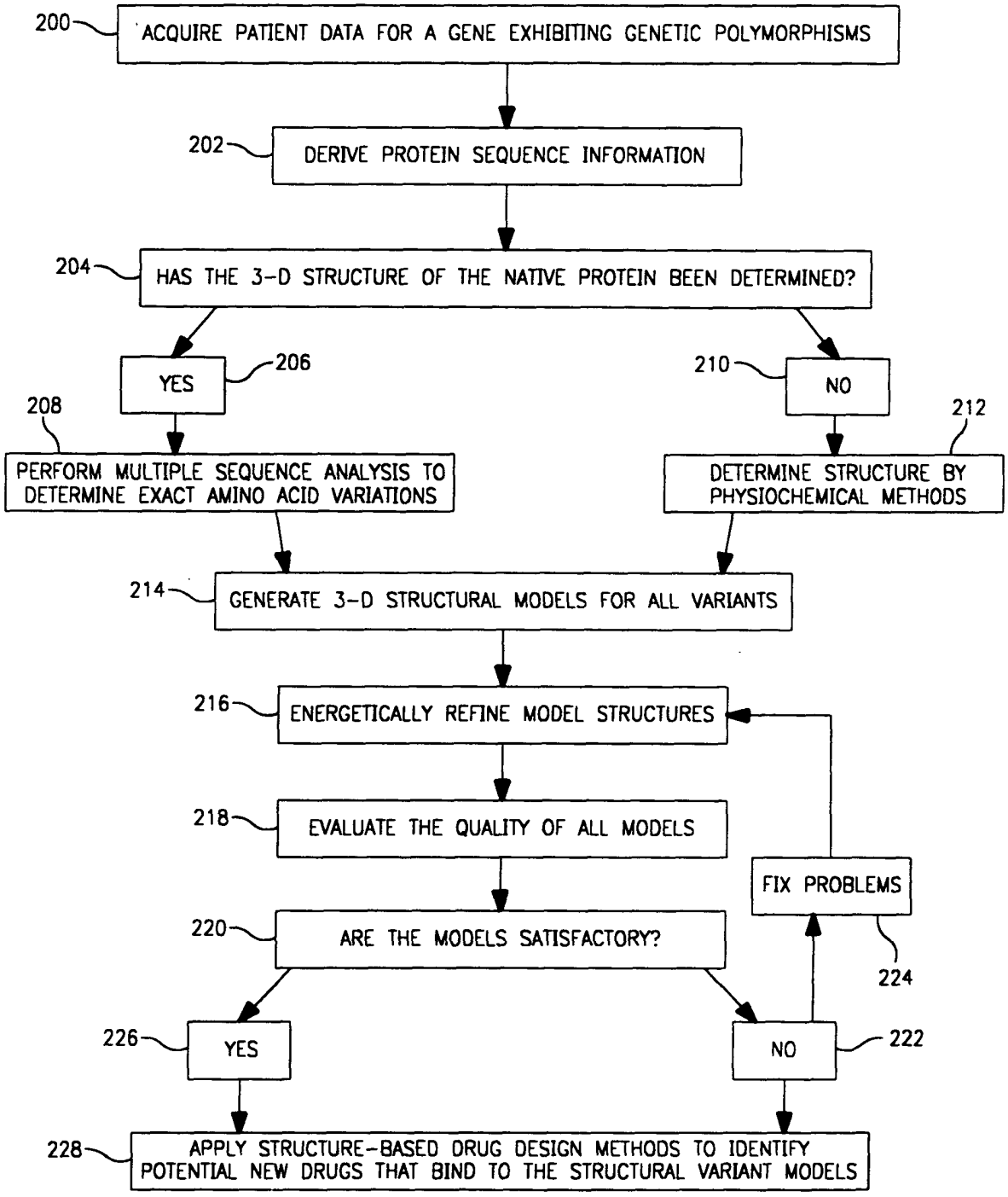



FIG. 2

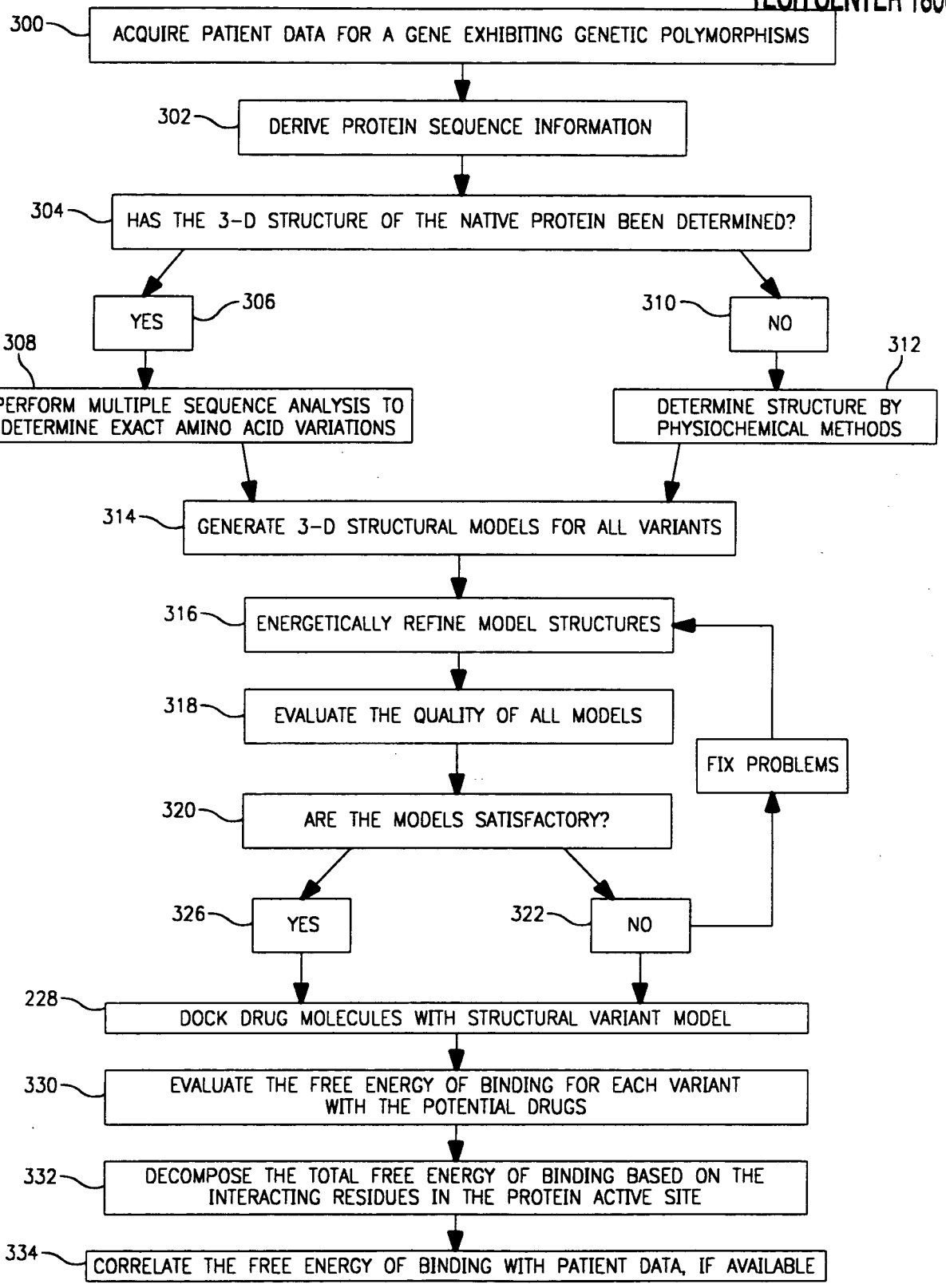



FIG. 3

COMPARISON OF CALCULATED VERUS EXPERIMENTAL BINDING FREE ENERGY CHANGES

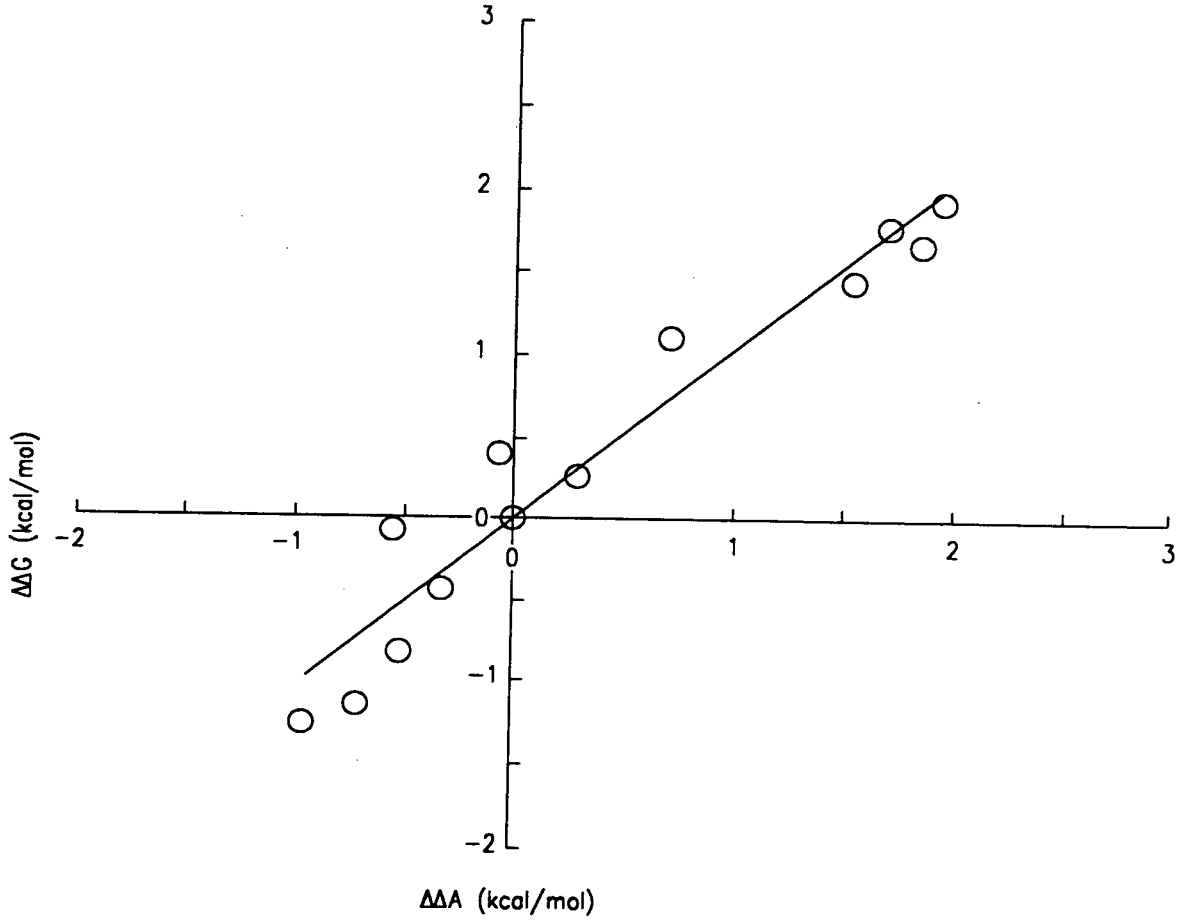



FIG. 5

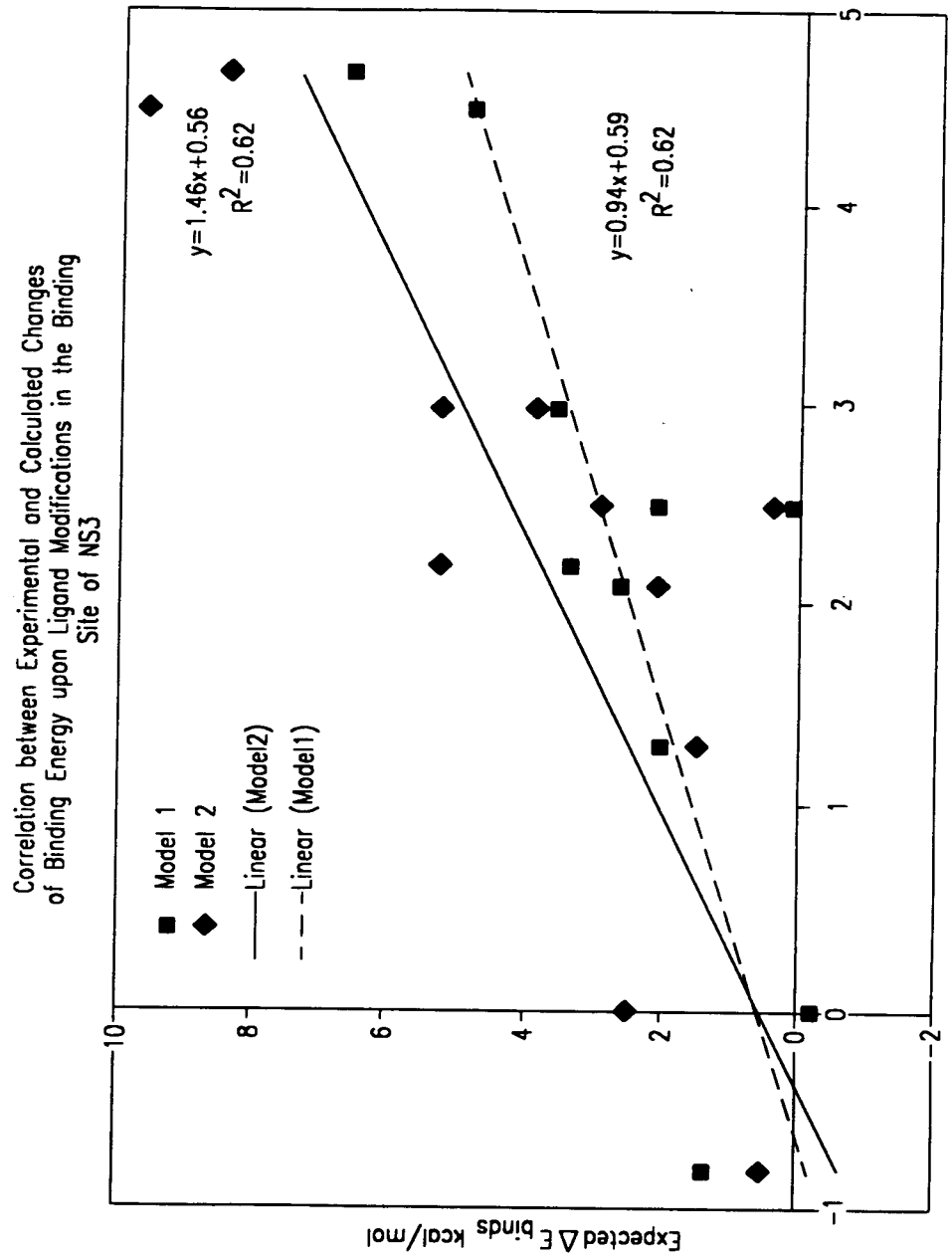
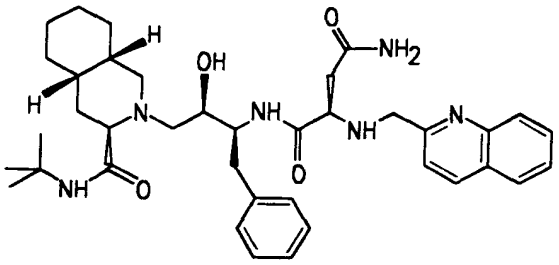
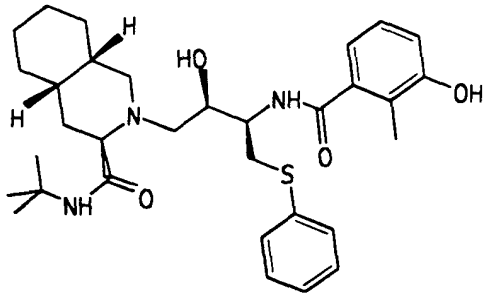



FIG. 4

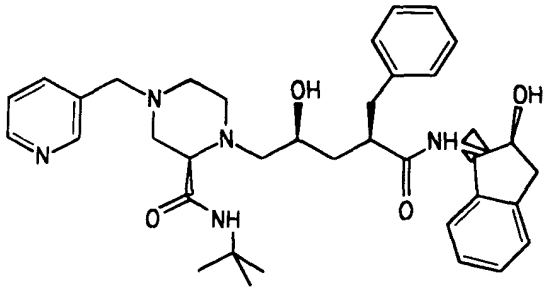
HIV PROTEASE INHIBITORS APPROVED BY FDA



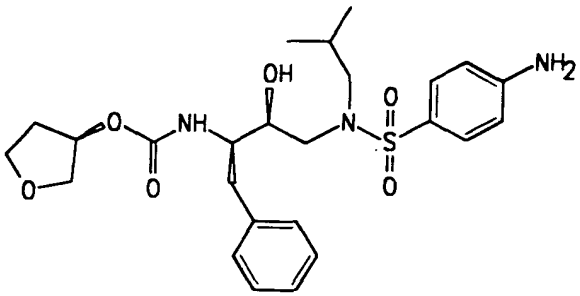
SAQUINAVIR



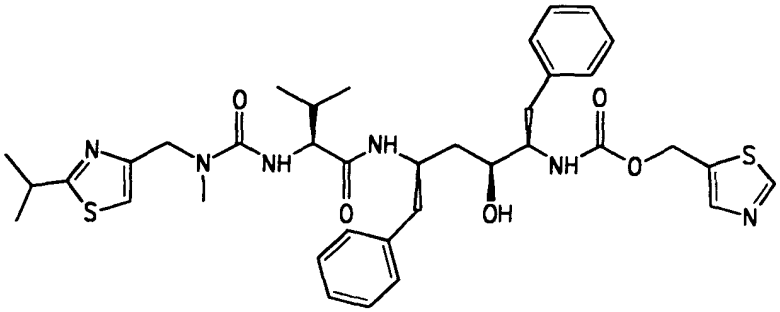
NELFINAVIR



INDINAVIR



AMPRENAVIR



RITONAVIR

FIG. 6

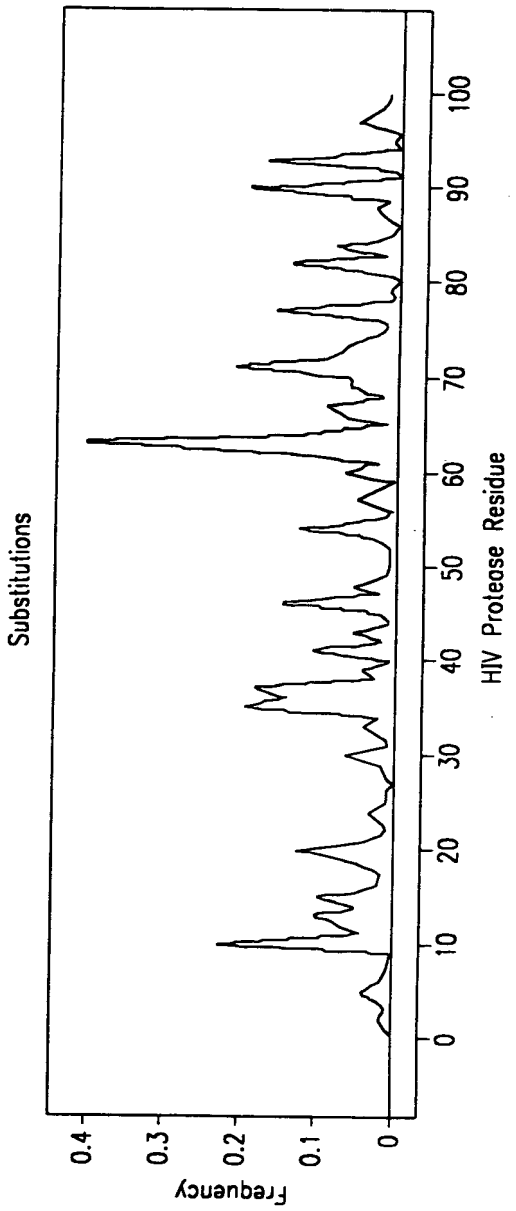



FIG. 7

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | PRO | A | 1 | -3.433 | 7.956 | 34.152 |
| ATOM | 2 | CA | PRO | A | 1 | -2.653 | 6.918 | 34.784 |
| ATOM | 3 | C | PRO | A | 1 | -1.242 | 7.005 | 34.259 |
| ATOM | 4 | O | PRO | A | 1 | -0.950 | 7.638 | 33.216 |
| ATOM | 5 | CB | PRO | A | 1 | -3.281 | 5.601 | 34.262 |
| ATOM | 6 | CG | PRO | A | 1 | -4.191 | 5.995 | 33.118 |
| ATOM | 7 | CD | PRO | A | 1 | -4.547 | 7.461 | 33.339 |
| ATOM | 8 | 1H | PRO | A | 1 | -2.845 | 8.493 | 33.547 |
| ATOM | 9 | 2H | PRO | A | 1 | -3.824 | 8.552 | 34.853 |
| ATOM | 10 | N | GLN | A | 2 | -0.259 | 6.464 | 35.001 |
| ATOM | 11 | H | GLN | A | 2 | -0.475 | 6.057 | 35.889 |
| ATOM | 12 | CA | GLN | A | 2 | 1.115 | 6.443 | 34.568 |
| ATOM | 13 | C | GLN | A | 2 | 1.452 | 4.993 | 34.301 |
| ATOM | 14 | O | GLN | A | 2 | 1.379 | 4.106 | 35.173 |
| ATOM | 15 | CB | GLN | A | 2 | 2.070 | 6.966 | 35.653 |
| ATOM | 16 | CG | GLN | A | 2 | 3.549 | 6.859 | 35.240 |
| ATOM | 17 | CD | GLN | A | 2 | 4.490 | 7.744 | 36.054 |
| ATOM | 18 | OE1 | GLN | A | 2 | 4.771 | 8.888 | 35.719 |
| ATOM | 19 | NE2 | GLN | A | 2 | 4.980 | 7.190 | 37.144 |
| ATOM | 20 | 1HE2 | GLN | A | 2 | 5.605 | 7.702 | 37.734 |
| ATOM | 21 | 2HE2 | GLN | A | 2 | 4.731 | 6.253 | 37.390 |
| ATOM | 22 | N | ILE | A | 3 | 1.784 | 4.644 | 33.037 |
| ATOM | 23 | H | ILE | A | 3 | 1.876 | 5.351 | 32.336 |
| ATOM | 24 | CA | ILE | A | 3 | 2.013 | 3.257 | 32.665 |
| ATOM | 25 | C | ILE | A | 3 | 3.505 | 3.028 | 32.473 |
| ATOM | 26 | O | ILE | A | 3 | 4.242 | 3.777 | 31.787 |
| ATOM | 27 | CB | ILE | A | 3 | 1.226 | 2.944 | 31.370 |
| ATOM | 28 | CG1 | ILE | A | 3 | -0.274 | 3.239 | 31.603 |
| ATOM | 29 | CG2 | ILE | A | 3 | 1.427 | 1.480 | 30.901 |
| ATOM | 30 | CD1 | ILE | A | 3 | -1.089 | 3.219 | 30.322 |
| ATOM | 31 | N | THR | A | 4 | 4.071 | 2.032 | 33.177 |
| ATOM | 32 | H | THR | A | 4 | 3.525 | 1.525 | 33.844 |
| ATOM | 33 | CA | THR | A | 4 | 5.451 | 1.661 | 33.007 |
| ATOM | 34 | C | THR | A | 4 | 5.515 | 0.637 | 31.901 |
| ATOM | 35 | O | THR | A | 4 | 4.490 | 0.143 | 31.397 |
| ATOM | 36 | CB | THR | A | 4 | 6.051 | 1.125 | 34.324 |
| ATOM | 37 | OG1 | THR | A | 4 | 5.224 | 0.069 | 34.791 |
| ATOM | 38 | HG1 | THR | A | 4 | 5.589 | -0.299 | 35.646 |
| ATOM | 39 | CG2 | THR | A | 4 | 6.085 | 2.212 | 35.431 |
| ATOM | 40 | N | LEU | A | 5 | 6.677 | 0.281 | 31.405 |
| ATOM | 41 | H | LEU | A | 5 | 7.518 | 0.530 | 31.885 |
| ATOM | 42 | CA | LEU | A | 5 | 6.754 | -0.464 | 30.177 |
| ATOM | 43 | C | LEU | A | 5 | 7.432 | -1.813 | 30.356 |
| ATOM | 44 | O | LEU | A | 5 | 7.940 | -2.464 | 29.426 |
| ATOM | 45 | CB | LEU | A | 5 | 7.459 | 0.394 | 29.128 |
| ATOM | 46 | CG | LEU | A | 5 | 6.668 | 1.671 | 28.775 |
| ATOM | 47 | CD1 | LEU | A | 5 | 7.493 | 2.649 | 27.939 |
| ATOM | 48 | CD2 | LEU | A | 5 | 5.345 | 1.307 | 28.099 |
| ATOM | 49 | N | TRP | A | 6 | 7.420 | -2.351 | 31.594 |
| ATOM | 50 | H | TRP | A | 6 | 7.030 | -1.833 | 32.356 |
| ATOM | 51 | CA | TRP | A | 6 | 7.958 | -3.669 | 31.865 |
| ATOM | 52 | C | TRP | A | 6 | 7.071 | -4.697 | 31.204 |
| ATOM | 53 | O | TRP | A | 6 | 7.520 | -5.798 | 30.828 |
| ATOM | 54 | CB | TRP | A | 6 | 8.099 | -3.913 | 33.367 |
| ATOM | 55 | CG | TRP | A | 6 | 9.041 | -2.974 | 34.070 |

FIG. 11A

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 56 | CD1 | TRP | A | 6 | 8.745 | -1.769 | 34.646 |
| ATOM | 57 | CD2 | TRP | A | 6 | 10.449 | -3.171 | 34.273 |
| ATOM | 58 | NE1 | TRP | A | 6 | 9.875 | -1.209 | 35.190 |
| ATOM | 59 | HE1 | TRP | A | 6 | 9.930 | -0.332 | 35.668 |
| ATOM | 60 | CE2 | TRP | A | 6 | 10.932 | -2.048 | 34.974 |
| ATOM | 61 | CE3 | TRP | A | 6 | 11.334 | -4.190 | 33.924 |
| ATOM | 62 | CZ2 | TRP | A | 6 | 12.257 | -1.917 | 35.333 |
| ATOM | 63 | CZ3 | TRP | A | 6 | 12.650 | -4.065 | 34.278 |
| ATOM | 64 | CH2 | TRP | A | 6 | 13.106 | -2.942 | 34.974 |
| ATOM | 65 | N | GLN | A | 7 | 5.773 | -4.448 | 30.973 |
| ATOM | 66 | H | GLN | A | 7 | 5.354 | -3.619 | 31.343 |
| ATOM | 67 | CA | GLN | A | 7 | 4.952 | -5.339 | 30.205 |
| ATOM | 68 | C | GLN | A | 7 | 4.438 | -4.569 | 29.033 |
| ATOM | 69 | O | GLN | A | 7 | 4.433 | -3.321 | 29.000 |
| ATOM | 70 | CB | GLN | A | 7 | 3.712 | -5.693 | 30.969 |
| ATOM | 71 | CG | GLN | A | 7 | 4.015 | -6.467 | 32.210 |
| ATOM | 72 | CD | GLN | A | 7 | 2.734 | -6.678 | 32.917 |
| ATOM | 73 | OE1 | GLN | A | 7 | 2.053 | -7.681 | 32.712 |
| ATOM | 74 | NE2 | GLN | A | 7 | 2.356 | -5.682 | 33.736 |
| ATOM | 75 | 1HE2 | GLN | A | 7 | 1.501 | -5.748 | 34.251 |
| ATOM | 76 | 2HE2 | GLN | A | 7 | 2.926 | -4.867 | 33.837 |
| ATOM | 77 | N | ARG | A | 8 | 3.777 | -5.239 | 28.078 |
| ATOM | 78 | H | ARG | A | 8 | 3.688 | -6.233 | 28.142 |
| ATOM | 79 | CA | ARG | A | 8 | 3.183 | -4.568 | 26.948 |
| ATOM | 80 | C | ARG | A | 8 | 2.117 | -3.648 | 27.461 |
| ATOM | 81 | O | ARG | A | 8 | 1.333 | -3.965 | 28.387 |
| ATOM | 82 | CB | ARG | A | 8 | 2.574 | -5.555 | 25.975 |
| ATOM | 83 | CG | ARG | A | 8 | 3.532 | -6.593 | 25.437 |
| ATOM | 84 | CD | ARG | A | 8 | 2.842 | -7.610 | 24.579 |
| ATOM | 85 | NE | ARG | A | 8 | 3.787 | -8.487 | 23.900 |
| ATOM | 86 | HE | ARG | A | 8 | 4.762 | -8.279 | 23.982 |
| ATOM | 87 | CZ | ARG | A | 8 | 3.405 | -9.541 | 23.185 |
| ATOM | 88 | NH1 | ARG | A | 8 | 2.125 | -9.871 | 23.052 |
| ATOM | 89 | 2HH1 | ARG | A | 8 | 1.418 | -9.321 | 23.496 |
| ATOM | 90 | 1HH1 | ARG | A | 8 | 1.869 | -10.670 | 22.508 |
| ATOM | 91 | NH2 | ARG | A | 8 | 4.332 | -10.286 | 22.589 |
| ATOM | 92 | 1HH2 | ARG | A | 8 | 4.062 | -11.082 | 22.048 |
| ATOM | 93 | 2HH2 | ARG | A | 8 | 5.299 | -10.050 | 22.682 |
| ATOM | 94 | N | PRO | A | 9 | 1.990 | -2.428 | 26.938 |
| ATOM | 95 | CA | PRO | A | 9 | 1.001 | -1.462 | 27.440 |
| ATOM | 96 | C | PRO | A | 9 | -0.365 | -1.697 | 26.821 |
| ATOM | 97 | O | PRO | A | 9 | -0.918 | -0.935 | 26.008 |
| ATOM | 98 | CB | PRO | A | 9 | 1.572 | -0.112 | 27.041 |
| ATOM | 99 | CG | PRO | A | 9 | 2.553 | -0.404 | 25.931 |
| ATOM | 100 | CD | PRO | A | 9 | 3.024 | -1.820 | 26.084 |
| ATOM | 101 | N | LEU | A | 10 | -1.028 | -2.803 | 27.227 |
| ATOM | 102 | H | LEU | A | 10 | -0.616 | -3.404 | 27.912 |
| ATOM | 103 | CA | LEU | A | 10 | -2.319 | -3.143 | 26.698 |
| ATOM | 104 | C | LEU | A | 10 | -3.390 | -2.565 | 27.591 |
| ATOM | 105 | O | LEU | A | 10 | -3.336 | -2.632 | 28.831 |
| ATOM | 106 | CB | LEU | A | 10 | -2.451 | -4.651 | 26.709 |
| ATOM | 107 | CG | LEU | A | 10 | -1.483 | -5.316 | 25.756 |
| ATOM | 108 | CD1 | LEU | A | 10 | -1.159 | -6.740 | 26.212 |
| ATOM | 109 | CD2 | LEU | A | 10 | -2.083 | -5.262 | 24.322 |
| ATOM | 110 | N | VAL | A | 11 | -4.447 | -1.952 | 27.033 |
| ATOM | 111 | H | VAL | A | 11 | -4.507 | -1.875 | 26.038 |

FIG. 1 IB

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 112 | CA | VAL | A | 11 | -5.506 | -1.398 | 27.835 |
| ATOM | 113 | C | VAL | A | 11 | -6.827 | -1.857 | 27.268 |
| ATOM | 114 | O | VAL | A | 11 | -6.924 | -2.490 | 26.198 |
| ATOM | 115 | CB | VAL | A | 11 | -5.420 | 0.143 | 27.897 |
| ATOM | 116 | CG1 | VAL | A | 11 | -4.117 | 0.595 | 28.551 |
| ATOM | 117 | CG2 | VAL | A | 11 | -5.549 | 0.787 | 26.497 |
| ATOM | 118 | N | THR | A | 12 | -7.954 | -1.592 | 27.978 |
| ATOM | 119 | H | THR | A | 12 | -7.884 | -1.141 | 28.868 |
| ATOM | 120 | CA | THR | A | 12 | -9.301 | -1.942 | 27.496 |
| ATOM | 121 | C | THR | A | 12 | -9.889 | -0.726 | 26.795 |
| ATOM | 122 | O | THR | A | 12 | -9.856 | 0.436 | 27.247 |
| ATOM | 123 | CB | THR | A | 12 | -10.225 | -2.385 | 28.659 |
| ATOM | 124 | OG1 | THR | A | 12 | -9.596 | -3.458 | 29.338 |
| ATOM | 125 | HG1 | THR | A | 12 | -10.170 | -3.766 | 30.096 |
| ATOM | 126 | CG2 | THR | A | 12 | -11.579 | -2.895 | 28.156 |
| ATOM | 127 | N | ILE | A | 13 | -10.449 | -0.932 | 25.594 |
| ATOM | 128 | H | ILE | A | 13 | -10.409 | -1.841 | 25.178 |
| ATOM | 129 | CA | ILE | A | 13 | -11.112 | 0.133 | 24.882 |
| ATOM | 130 | C | ILE | A | 13 | -12.553 | -0.292 | 24.693 |
| ATOM | 131 | O | ILE | A | 13 | -12.935 | -1.469 | 24.821 |
| ATOM | 132 | CB | ILE | A | 13 | -10.432 | 0.364 | 23.511 |
| ATOM | 133 | CG1 | ILE | A | 13 | -10.466 | -0.896 | 22.628 |
| ATOM | 134 | CG2 | ILE | A | 13 | -8.986 | 0.806 | 23.747 |
| ATOM | 135 | CD1 | ILE | A | 13 | -9.755 | -0.745 | 21.294 |
| ATOM | 136 | N | LYS | A | 14 | -13.470 | 0.658 | 24.438 |
| ATOM | 137 | H | LYS | A | 14 | -13.209 | 1.622 | 24.481 |
| ATOM | 138 | CA | LYS | A | 14 | -14.838 | 0.330 | 24.100 |
| ATOM | 139 | C | LYS | A | 14 | -15.088 | 0.877 | 22.719 |
| ATOM | 140 | O | LYS | A | 14 | -14.859 | 2.059 | 22.375 |
| ATOM | 141 | CB | LYS | A | 14 | -15.855 | 0.916 | 25.099 |
| ATOM | 142 | CG | LYS | A | 14 | -17.325 | 0.518 | 24.864 |
| ATOM | 143 | CD | LYS | A | 14 | -18.078 | 0.146 | 26.166 |
| ATOM | 144 | CE | LYS | A | 14 | -18.826 | 1.342 | 26.810 |
| ATOM | 145 | NZ | LYS | A | 14 | -19.316 | 0.929 | 28.173 |
| ATOM | 146 | 1HZ | LYS | A | 14 | -19.801 | 1.693 | 28.599 |
| ATOM | 147 | 3HZ | LYS | A | 14 | -18.536 | 0.670 | 28.743 |
| ATOM | 148 | 2HZ | LYS | A | 14 | -19.936 | 0.150 | 28.082 |
| ATOM | 149 | N | ILE | A | 15 | -15.535 | 0.005 | 21.798 |
| ATOM | 150 | H | ILE | A | 15 | -15.806 | -0.916 | 22.078 |
| ATOM | 151 | CA | ILE | A | 15 | -15.642 | 0.347 | 20.400 |
| ATOM | 152 | C | ILE | A | 15 | -16.894 | -0.328 | 19.887 |
| ATOM | 153 | O | ILE | A | 15 | -17.115 | -1.542 | 20.041 |
| ATOM | 154 | CB | ILE | A | 15 | -14.382 | -0.132 | 19.639 |
| ATOM | 155 | CG1 | ILE | A | 15 | -14.478 | 0.148 | 18.125 |
| ATOM | 156 | CG2 | ILE | A | 15 | -14.082 | -1.623 | 19.880 |
| ATOM | 157 | CD1 | ILE | A | 15 | -14.237 | 1.603 | 17.796 |
| ATOM | 158 | N | GLY | A | 16 | -17.843 | 0.435 | 19.308 |
| ATOM | 159 | H | GLY | A | 16 | -17.720 | 1.426 | 19.260 |
| ATOM | 160 | CA | GLY | A | 16 | -19.053 | -0.143 | 18.745 |
| ATOM | 161 | C | GLY | A | 16 | -19.897 | -0.817 | 19.789 |
| ATOM | 162 | O | GLY | A | 16 | -20.774 | -1.668 | 19.516 |
| ATOM | 163 | N | GLY | A | 17 | -19.712 | -0.493 | 21.088 |
| ATOM | 164 | H | GLY | A | 17 | -19.038 | 0.204 | 21.334 |
| ATOM | 165 | CA | GLY | A | 17 | -20.464 | -1.126 | 22.160 |
| ATOM | 166 | C | GLY | A | 17 | -19.718 | -2.335 | 22.653 |
| ATOM | 167 | O | GLY | A | 17 | -20.147 | -3.098 | 23.540 |

FIG. 1IC

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 168 | N | GLN | A | 18 | -18.507 | -2.591 | 22.121 |
| ATOM | 169 | H | GLN | A | 18 | -18.059 | -1.900 | 21.554 |
| ATOM | 170 | CA | GLN | A | 18 | -17.806 | -3.830 | 22.326 |
| ATOM | 171 | C | GLN | A | 18 | -16.552 | -3.549 | 23.123 |
| ATOM | 172 | O | GLN | A | 18 | -15.887 | -2.508 | 22.945 |
| ATOM | 173 | CB | GLN | A | 18 | -17.393 | -4.294 | 20.928 |
| ATOM | 174 | CG | GLN | A | 18 | -16.911 | -5.734 | 20.788 |
| ATOM | 175 | CD | GLN | A | 18 | -18.018 | -6.728 | 20.613 |
| ATOM | 176 | OE1 | GLN | A | 18 | -19.131 | -6.574 | 21.152 |
| ATOM | 177 | NE2 | GLN | A | 18 | -17.722 | -7.773 | 19.857 |
| ATOM | 178 | 1HE2 | GLN | A | 18 | -18.404 | -8.484 | 19.689 |
| ATOM | 179 | 2HE2 | GLN | A | 18 | -16.814 | -7.860 | 19.448 |
| ATOM | 180 | N | LEU | A | 19 | -16.133 | -4.397 | 24.087 |
| ATOM | 181 | H | LEU | A | 19 | -16.682 | -5.202 | 24.312 |
| ATOM | 182 | CA | LEU | A | 19 | -14.909 | -4.178 | 24.808 |
| ATOM | 183 | C | LEU | A | 19 | -13.799 | -4.912 | 24.090 |
| ATOM | 184 | O | LEU | A | 19 | -13.989 | -6.018 | 23.558 |
| ATOM | 185 | CB | LEU | A | 19 | -14.982 | -4.714 | 26.254 |
| ATOM | 186 | CG | LEU | A | 19 | -15.490 | -3.778 | 27.374 |
| ATOM | 187 | CD1 | LEU | A | 19 | -16.392 | -2.639 | 26.856 |
| ATOM | 188 | CD2 | LEU | A | 19 | -16.208 | -4.516 | 28.465 |
| ATOM | 189 | N | LYS | A | 20 | -12.603 | -4.372 | 23.978 |
| ATOM | 190 | H | LYS | A | 20 | -12.442 | -3.448 | 24.324 |
| ATOM | 191 | CA | LYS | A | 20 | -11.507 | -5.082 | 23.365 |
| ATOM | 192 | C | LYS | A | 20 | -10.266 | -4.618 | 24.062 |
| ATOM | 193 | O | LYS | A | 20 | -10.228 | -3.611 | 24.816 |
| ATOM | 194 | CB | LYS | A | 20 | -11.397 | -4.798 | 21.875 |
| ATOM | 195 | CG | LYS | A | 20 | -12.558 | -5.356 | 21.100 |
| ATOM | 196 | CD | LYS | A | 20 | -12.537 | -4.988 | 19.615 |
| ATOM | 197 | CE | LYS | A | 20 | -13.414 | -5.958 | 18.827 |
| ATOM | 198 | NZ | LYS | A | 20 | -12.681 | -7.208 | 18.639 |
| ATOM | 199 | 1HZ | LYS | A | 20 | -13.247 | -7.852 | 18.123 |
| ATOM | 200 | 3HZ | LYS | A | 20 | -12.458 | -7.601 | 19.531 |
| ATOM | 201 | 2HZ | LYS | A | 20 | -11.837 | -7.027 | 18.134 |
| ATOM | 202 | N | GLU | A | 21 | -9.150 | -5.357 | 23.893 |
| ATOM | 203 | H | GLU | A | 21 | -9.185 | -6.188 | 23.338 |
| ATOM | 204 | CA | GLU | A | 21 | -7.890 | -4.997 | 24.486 |
| ATOM | 205 | C | GLU | A | 21 | -7.001 | -4.462 | 23.390 |
| ATOM | 206 | O | GLU | A | 21 | -6.970 | -4.992 | 22.258 |
| ATOM | 207 | CB | GLU | A | 21 | -7.268 | -6.260 | 25.051 |
| ATOM | 208 | CG | GLU | A | 21 | -5.835 | -6.140 | 25.480 |
| ATOM | 209 | CD | GLU | A | 21 | -5.405 | -7.352 | 26.275 |
| ATOM | 210 | OE1 | GLU | A | 21 | -5.624 | -7.343 | 27.508 |
| ATOM | 211 | OE2 | GLU | A | 21 | -4.852 | -8.309 | 25.684 |
| ATOM | 212 | N | ALA | A | 22 | -6.239 | -3.369 | 23.595 |
| ATOM | 213 | H | ALA | A | 22 | -6.223 | -2.938 | 24.497 |
| ATOM | 214 | CA | ALA | A | 22 | -5.419 | -2.781 | 22.520 |
| ATOM | 215 | C | ALA | A | 22 | -4.138 | -2.255 | 23.114 |
| ATOM | 216 | O | ALA | A | 22 | -3.985 | -1.914 | 24.314 |
| ATOM | 217 | CB | ALA | A | 22 | -6.134 | -1.657 | 21.821 |
| ATOM | 218 | N | LEU | A | 23 | -3.121 | -2.091 | 22.240 |
| ATOM | 219 | H | LEU | A | 23 | -3.279 | -2.236 | 21.263 |
| ATOM | 220 | CA | LEU | A | 23 | -1.797 | -1.712 | 22.640 |
| ATOM | 221 | C | LEU | A | 23 | -1.660 | -0.230 | 22.443 |
| ATOM | 222 | O | LEU | A | 23 | -2.020 | 0.349 | 21.402 |
| ATOM | 223 | CB | LEU | A | 23 | -0.814 | -2.486 | 21.732 |

FIG. 11D

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 224 | CG | LEU | A | 23 | 0.705 | -2.448 | 21.991 |
| ATOM | 225 | CD1 | LEU | A | 23 | 1.088 | -3.400 | 23.124 |
| ATOM | 226 | CD2 | LEU | A | 23 | 1.462 | -2.878 | 20.708 |
| ATOM | 227 | N | LEU | A | 24 | -1.192 | 0.530 | 23.463 |
| ATOM | 228 | H | LEU | A | 24 | -1.015 | 0.110 | 24.353 |
| ATOM | 229 | CA | LEU | A | 24 | -0.935 | 1.952 | 23.305 |
| ATOM | 230 | C | LEU | A | 24 | 0.403 | 2.089 | 22.609 |
| ATOM | 231 | O | LEU | A | 24 | 1.471 | 1.717 | 23.130 |
| ATOM | 232 | CB | LEU | A | 24 | -0.921 | 2.609 | 24.681 |
| ATOM | 233 | CG | LEU | A | 24 | -2.220 | 2.492 | 25.477 |
| ATOM | 234 | CD1 | LEU | A | 24 | -2.063 | 3.291 | 26.772 |
| ATOM | 235 | CD2 | LEU | A | 24 | -3.419 | 3.000 | 24.691 |
| ATOM | 236 | N | ASP | A | 25 | 0.454 | 2.590 | 21.397 |
| ATOM | 237 | H | ASP | A | 25 | -0.334 | 3.085 | 21.032 |
| ATOM | 238 | CA | ASP | A | 25 | 1.642 | 2.423 | 20.605 |
| ATOM | 239 | C | ASP | A | 25 | 2.130 | 3.750 | 20.059 |
| ATOM | 240 | O | ASP | A | 25 | 1.568 | 4.320 | 19.110 |
| ATOM | 241 | CB | ASP | A | 25 | 1.263 | 1.435 | 19.486 |
| ATOM | 242 | CG | ASP | A | 25 | 2.428 | 1.051 | 18.561 |
| ATOM | 243 | OD1 | ASP | A | 25 | 3.546 | 1.540 | 18.729 |
| ATOM | 244 | OD2 | ASP | A | 25 | 2.164 | 0.241 | 17.658 |
| ATOM | 245 | N | THR | A | 26 | 3.203 | 4.337 | 20.605 |
| ATOM | 246 | H | THR | A | 26 | 3.694 | 3.880 | 21.346 |
| ATOM | 247 | CA | THR | A | 26 | 3.691 | 5.652 | 20.144 |
| ATOM | 248 | C | THR | A | 26 | 4.397 | 5.583 | 18.778 |
| ATOM | 249 | O | THR | A | 26 | 4.642 | 6.587 | 18.079 |
| ATOM | 250 | CB | THR | A | 26 | 4.596 | 6.219 | 21.217 |
| ATOM | 251 | OG1 | THR | A | 26 | 5.716 | 5.324 | 21.386 |
| ATOM | 252 | HG1 | THR | A | 26 | 6.332 | 5.676 | 22.091 |
| ATOM | 253 | CG2 | THR | A | 26 | 3.878 | 6.320 | 22.577 |
| ATOM | 254 | N | GLY | A | 27 | 4.757 | 4.377 | 18.298 |
| ATOM | 255 | H | GLY | A | 27 | 4.526 | 3.550 | 18.811 |
| ATOM | 256 | CA | GLY | A | 27 | 5.481 | 4.233 | 17.040 |
| ATOM | 257 | C | GLY | A | 27 | 4.520 | 4.190 | 15.886 |
| ATOM | 258 | O | GLY | A | 27 | 4.908 | 4.242 | 14.696 |
| ATOM | 259 | N | ALA | A | 28 | 3.197 | 4.084 | 16.117 |
| ATOM | 260 | H | ALA | A | 28 | 2.856 | 4.091 | 17.057 |
| ATOM | 261 | CA | ALA | A | 28 | 2.213 | 3.955 | 15.018 |
| ATOM | 262 | C | ALA | A | 28 | 1.598 | 5.299 | 14.750 |
| ATOM | 263 | O | ALA | A | 28 | 1.062 | 5.982 | 15.650 |
| ATOM | 264 | CB | ALA | A | 28 | 1.117 | 2.980 | 15.390 |
| ATOM | 265 | N | ASP | A | 29 | 1.503 | 5.744 | 13.490 |
| ATOM | 266 | H | ASP | A | 29 | 1.912 | 5.216 | 12.746 |
| ATOM | 267 | CA | ASP | A | 29 | 0.810 | 6.984 | 13.213 |
| ATOM | 268 | C | ASP | A | 29 | -0.666 | 6.724 | 13.327 |
| ATOM | 269 | O | ASP | A | 29 | -1.488 | 7.637 | 13.568 |
| ATOM | 270 | CB | ASP | A | 29 | 1.009 | 7.433 | 11.775 |
| ATOM | 271 | CG | ASP | A | 29 | 2.439 | 7.882 | 11.412 |
| ATOM | 272 | OD1 | ASP | A | 29 | 3.360 | 7.856 | 12.269 |
| ATOM | 273 | OD2 | ASP | A | 29 | 2.606 | 8.253 | 10.252 |
| ATOM | 274 | N | ASP | A | 30 | -1.143 | 5.517 | 12.990 |
| ATOM | 275 | H | ASP | A | 30 | -0.508 | 4.769 | 12.800 |
| ATOM | 276 | CA | ASP | A | 30 | -2.579 | 5.245 | 12.887 |
| ATOM | 277 | C | ASP | A | 30 | -3.057 | 4.208 | 13.867 |
| ATOM | 278 | O | ASP | A | 30 | -2.284 | 3.483 | 14.546 |
| ATOM | 279 | CB | ASP | A | 30 | -2.896 | 4.758 | 11.456 |

FIG. 1E

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 280 | CG | ASP | A | 30 | -2.495 | 5.768 | 10.425 |
| ATOM | 281 | OD1 | ASP | A | 30 | -3.067 | 6.871 | 10.423 |
| ATOM | 282 | OD2 | ASP | A | 30 | -1.596 | 5.494 | 9.618 |
| ATOM | 283 | N | THR | A | 31 | -4.393 | 4.076 | 14.002 |
| ATOM | 284 | H | THR | A | 31 | -5.004 | 4.700 | 13.515 |
| ATOM | 285 | CA | THR | A | 31 | -5.059 | 3.062 | 14.829 |
| ATOM | 286 | C | THR | A | 31 | -5.565 | 1.967 | 13.913 |
| ATOM | 287 | O | THR | A | 31 | -6.223 | 2.169 | 12.870 |
| ATOM | 288 | CB | THR | A | 31 | -6.212 | 3.725 | 15.566 |
| ATOM | 289 | OG1 | THR | A | 31 | -5.668 | 4.667 | 16.474 |
| ATOM | 290 | HG1 | THR | A | 31 | -6.403 | 5.122 | 16.976 |
| ATOM | 291 | CG2 | THR | A | 31 | -7.044 | 2.702 | 16.389 |
| ATOM | 292 | N | VAL | A | 32 | -5.187 | 0.713 | 14.235 |
| ATOM | 293 | H | VAL | A | 32 | -4.649 | 0.555 | 15.063 |
| ATOM | 294 | CA | VAL | A | 32 | -5.517 | -0.462 | 13.437 |
| ATOM | 295 | C | VAL | A | 32 | -6.092 | -1.506 | 14.365 |
| ATOM | 296 | O | VAL | A | 32 | -5.502 | -1.957 | 15.365 |
| ATOM | 297 | CB | VAL | A | 32 | -4.260 | -1.064 | 12.757 |
| ATOM | 298 | CG1 | VAL | A | 32 | -4.667 | -2.136 | 11.735 |
| ATOM | 299 | CG2 | VAL | A | 32 | -3.422 | 0.017 | 12.032 |
| ATOM | 300 | N | LEU | A | 33 | -7.352 | -1.923 | 14.119 |
| ATOM | 301 | H | LEU | A | 33 | -7.867 | -1.523 | 13.361 |
| ATOM | 302 | CA | LEU | A | 33 | -7.982 | -2.940 | 14.929 |
| ATOM | 303 | C | LEU | A | 33 | -8.174 | -4.203 | 14.107 |
| ATOM | 304 | O | LEU | A | 33 | -8.268 | -4.247 | 12.853 |
| ATOM | 305 | CB | LEU | A | 33 | -9.336 | -2.477 | 15.408 |
| ATOM | 306 | CG | LEU | A | 33 | -9.292 | -1.149 | 16.127 |
| ATOM | 307 | CD1 | LEU | A | 33 | -10.710 | -0.747 | 16.485 |
| ATOM | 308 | CD2 | LEU | A | 33 | -8.348 | -1.139 | 17.347 |
| ATOM | 309 | N | GLU | A | 34 | -8.296 | -5.319 | 14.782 |
| ATOM | 310 | H | GLU | A | 34 | -8.244 | -5.302 | 15.780 |
| ATOM | 311 | CA | GLU | A | 34 | -8.503 | -6.551 | 14.086 |
| ATOM | 312 | C | GLU | A | 34 | -9.909 | -6.549 | 13.510 |
| ATOM | 313 | O | GLU | A | 34 | -10.808 | -5.717 | 13.795 |
| ATOM | 314 | CB | GLU | A | 34 | -8.265 | -7.750 | 15.010 |
| ATOM | 315 | CG | GLU | A | 34 | -9.259 | -7.791 | 16.165 |
| ATOM | 316 | CD | GLU | A | 34 | -8.763 | -8.552 | 17.404 |
| ATOM | 317 | OE1 | GLU | A | 34 | -7.670 | -9.193 | 17.368 |
| ATOM | 318 | OE2 | GLU | A | 34 | -9.482 | -8.497 | 18.407 |
| ATOM | 319 | N | GLU | A | 35 | -10.152 | -7.480 | 12.568 |
| ATOM | 320 | H | GLU | A | 35 | -9.485 | -8.208 | 12.407 |
| ATOM | 321 | CA | GLU | A | 35 | -11.352 | -7.466 | 11.773 |
| ATOM | 322 | C | GLU | A | 35 | -12.631 | -7.520 | 12.571 |
| ATOM | 323 | O | GLU | A | 35 | -12.814 | -8.294 | 13.528 |
| ATOM | 324 | CB | GLU | A | 35 | -11.237 | -8.536 | 10.707 |
| ATOM | 325 | CG | GLU | A | 35 | -9.945 | -8.280 | 9.907 |
| ATOM | 326 | CD | GLU | A | 35 | -9.872 | -8.872 | 8.486 |
| ATOM | 327 | OE1 | GLU | A | 35 | -10.612 | -8.401 | 7.603 |
| ATOM | 328 | OE2 | GLU | A | 35 | -9.024 | -9.776 | 8.261 |
| ATOM | 329 | N | MET | A | 36 | -13.580 | -6.598 | 12.278 |
| ATOM | 330 | H | MET | A | 36 | -13.439 | -5.967 | 11.515 |
| ATOM | 331 | CA | MET | A | 36 | -14.819 | -6.495 | 13.052 |
| ATOM | 332 | C | MET | A | 36 | -15.826 | -5.635 | 12.271 |
| ATOM | 333 | O | MET | A | 36 | -15.514 | -4.828 | 11.371 |
| ATOM | 334 | CB | MET | A | 36 | -14.593 | -5.845 | 14.428 |
| ATOM | 335 | CG | MET | A | 36 | -14.279 | -4.353 | 14.417 |

FIG. 1F

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 336 | SD | MET | A | 36 | -14.251 | -3.718 | 16.099 |
| ATOM | 337 | CE | MET | A | 36 | -12.487 | -3.846 | 16.409 |
| ATOM | 338 | N | SER | A | 37 | -17.130 | -5.776 | 12.590 |
| ATOM | 339 | H | SER | A | 37 | -17.399 | -6.431 | 13.296 |
| ATOM | 340 | CA | SER | A | 37 | -18.155 | -5.005 | 11.940 |
| ATOM | 341 | C | SER | A | 37 | -18.286 | -3.693 | 12.657 |
| ATOM | 342 | O | SER | A | 37 | -18.593 | -3.624 | 13.865 |
| ATOM | 343 | CB | SER | A | 37 | -19.506 | -5.688 | 12.032 |
| ATOM | 344 | OG | SER | A | 37 | -19.455 | -7.054 | 11.716 |
| ATOM | 345 | HG | SER | A | 37 | -20.367 | -7.457 | 11.791 |
| ATOM | 346 | N | LEU | A | 38 | -18.185 | -2.569 | 11.933 |
| ATOM | 347 | H | LEU | A | 38 | -17.956 | -2.625 | 10.952 |
| ATOM | 348 | CA | LEU | A | 38 | -18.557 | -1.247 | 12.465 |
| ATOM | 349 | C | LEU | A | 38 | -19.630 | -0.605 | 11.572 |
| ATOM | 350 | O | LEU | A | 38 | -19.706 | -0.939 | 10.391 |
| ATOM | 351 | CB | LEU | A | 38 | -17.315 | -0.346 | 12.588 |
| ATOM | 352 | CG | LEU | A | 38 | -16.246 | -0.818 | 13.596 |
| ATOM | 353 | CD1 | LEU | A | 38 | -14.998 | 0.073 | 13.489 |
| ATOM | 354 | CD2 | LEU | A | 38 | -16.756 | -0.787 | 15.046 |
| ATOM | 355 | N | PRO | A | 39 | -20.455 | 0.321 | 12.108 |
| ATOM | 356 | CA | PRO | A | 39 | -21.460 | 1.053 | 11.339 |
| ATOM | 357 | C | PRO | A | 39 | -20.824 | 2.176 | 10.502 |
| ATOM | 358 | O | PRO | A | 39 | -19.654 | 2.519 | 10.685 |
| ATOM | 359 | CB | PRO | A | 39 | -22.430 | 1.607 | 12.389 |
| ATOM | 360 | CG | PRO | A | 39 | -21.531 | 1.845 | 13.600 |
| ATOM | 361 | CD | PRO | A | 39 | -20.539 | 0.686 | 13.517 |
| ATOM | 362 | N | GLY | A | 40 | -21.620 | 2.749 | 9.586 |
| ATOM | 363 | H | GLY | A | 40 | -22.569 | 2.417 | 9.493 |
| ATOM | 364 | CA | GLY | A | 40 | -21.203 | 3.811 | 8.678 |
| ATOM | 365 | C | GLY | A | 40 | -20.836 | 3.262 | 7.298 |
| ATOM | 366 | O | GLY | A | 40 | -21.405 | 2.268 | 6.845 |
| ATOM | 367 | N | LYS | A | 41 | -19.895 | 3.945 | 6.631 |
| ATOM | 368 | H | LYS | A | 41 | -19.496 | 4.761 | 7.071 |
| ATOM | 369 | CA | LYS | A | 41 | -19.323 | 3.558 | 5.343 |
| ATOM | 370 | C | LYS | A | 41 | -17.798 | 3.757 | 5.371 |
| ATOM | 371 | O | LYS | A | 41 | -17.263 | 4.462 | 6.229 |
| ATOM | 372 | CB | LYS | A | 41 | -20.025 | 4.352 | 4.224 |
| ATOM | 373 | CG | LYS | A | 41 | -19.703 | 3.839 | 2.810 |
| ATOM | 374 | CD | LYS | A | 41 | -20.610 | 4.486 | 1.757 |
| ATOM | 375 | CE | LYS | A | 41 | -20.240 | 3.964 | 0.366 |
| ATOM | 376 | NZ | LYS | A | 41 | -21.097 | 4.552 | -0.678 |
| ATOM | 377 | 1HZ | LYS | A | 41 | -20.824 | 4.189 | -1.580 |
| ATOM | 378 | 3HZ | LYS | A | 41 | -20.993 | 5.556 | -0.673 |
| ATOM | 379 | 2HZ | LYS | A | 41 | -22.061 | 4.311 | -0.498 |
| ATOM | 380 | N | TRP | A | 42 | -17.104 | 3.091 | 4.439 |
| ATOM | 381 | H | TRP | A | 42 | -17.620 | 2.548 | 3.762 |
| ATOM | 382 | CA | TRP | A | 42 | -15.654 | 2.932 | 4.423 |
| ATOM | 383 | C | TRP | A | 42 | -15.105 | 2.852 | 2.994 |
| ATOM | 384 | O | TRP | A | 42 | -15.845 | 2.702 | 2.021 |
| ATOM | 385 | CB | TRP | A | 42 | -15.279 | 1.675 | 5.236 |
| ATOM | 386 | CG | TRP | A | 42 | -16.214 | 0.514 | 5.094 |
| ATOM | 387 | CD1 | TRP | A | 42 | -16.230 | -0.402 | 4.101 |
| ATOM | 388 | CD2 | TRP | A | 42 | -17.355 | 0.203 | 5.942 |
| ATOM | 389 | NE1 | TRP | A | 42 | -17.297 | -1.260 | 4.281 |
| ATOM | 390 | HE1 | TRP | A | 42 | -17.504 | -2.015 | 3.644 |
| ATOM | 391 | CE2 | TRP | A | 42 | -18.045 | -0.914 | 5.389 |

FIG. 11G

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 392 | CE3 | TRP | A | 42 | -17.896 | 0.792 | 7.103 |
| ATOM | 393 | CZ2 | TRP | A | 42 | -19.224 | -1.421 | 5.959 |
| ATOM | 394 | CZ3 | TRP | A | 42 | -19.077 | 0.298 | 7.675 |
| ATOM | 395 | CH2 | TRP | A | 42 | -19.741 | -0.806 | 7.112 |
| ATOM | 396 | N | LYS | A | 43 | -13.771 | 2.932 | 2.911 |
| ATOM | 397 | H | LYS | A | 43 | -13.260 | 3.058 | 3.773 |
| ATOM | 398 | CA | LYS | A | 43 | -12.951 | 2.802 | 1.713 |
| ATOM | 399 | C | LYS | A | 43 | -11.773 | 1.859 | 2.012 |
| ATOM | 400 | O | LYS | A | 43 | -11.359 | 1.760 | 3.166 |
| ATOM | 401 | CB | LYS | A | 43 | -12.451 | 4.193 | 1.270 |
| ATOM | 402 | CG | LYS | A | 43 | -11.724 | 4.979 | 2.383 |
| ATOM | 403 | CD | LYS | A | 43 | -11.060 | 6.267 | 1.873 |
| ATOM | 404 | CE | LYS | A | 43 | -9.784 | 6.001 | 1.065 |
| ATOM | 405 | NZ | LYS | A | 43 | -8.700 | 5.458 | 1.903 |
| ATOM | 406 | 1HZ | LYS | A | 43 | -7.876 | 5.315 | 1.338 |
| ATOM | 407 | 3HZ | LYS | A | 43 | -8.993 | 4.576 | 2.300 |
| ATOM | 408 | 2HZ | LYS | A | 43 | -8.493 | 6.108 | 2.647 |
| ATOM | 409 | N | PRO | A | 44 | -11.177 | 1.197 | 1.004 |
| ATOM | 410 | CA | PRO | A | 44 | -9.947 | 0.435 | 1.187 |
| ATOM | 411 | C | PRO | A | 44 | -8.760 | 1.392 | 1.379 |
| ATOM | 412 | O | PRO | A | 44 | -8.711 | 2.434 | 0.720 |
| ATOM | 413 | CB | PRO | A | 44 | -9.808 | -0.393 | -0.095 |
| ATOM | 414 | CG | PRO | A | 44 | -10.501 | 0.458 | -1.159 |
| ATOM | 415 | CD | PRO | A | 44 | -11.630 | 1.132 | -0.380 |
| ATOM | 416 | N | LYS | A | 45 | -7.790 | 1.030 | 2.240 |
| ATOM | 417 | H | LYS | A | 45 | -7.912 | 0.227 | 2.824 |
| ATOM | 418 | CA | LYS | A | 45 | -6.547 | 1.747 | 2.314 |
| ATOM | 419 | C | LYS | A | 45 | -5.493 | 0.683 | 2.507 |
| ATOM | 420 | O | LYS | A | 45 | -5.780 | -0.470 | 2.869 |
| ATOM | 421 | CB | LYS | A | 45 | -6.594 | 2.699 | 3.524 |
| ATOM | 422 | CG | LYS | A | 45 | -5.463 | 3.744 | 3.609 |
| ATOM | 423 | CD | LYS | A | 45 | -5.340 | 4.289 | 5.052 |
| ATOM | 424 | CE | LYS | A | 45 | -4.262 | 5.383 | 5.204 |
| ATOM | 425 | NZ | LYS | A | 45 | -2.907 | 4.911 | 4.916 |
| ATOM | 426 | 1HZ | LYS | A | 45 | -2.260 | 5.664 | 5.032 |
| ATOM | 427 | 3HZ | LYS | A | 45 | -2.864 | 4.577 | 3.975 |
| ATOM | 428 | 2HZ | LYS | A | 45 | -2.672 | 4.169 | 5.544 |
| ATOM | 429 | N | MET | A | 46 | -4.224 | 0.949 | 2.193 |
| ATOM | 430 | H | MET | A | 46 | -3.998 | 1.805 | 1.728 |
| ATOM | 431 | CA | MET | A | 46 | -3.157 | 0.027 | 2.509 |
| ATOM | 432 | C | MET | A | 46 | -2.417 | 0.701 | 3.627 |
| ATOM | 433 | O | MET | A | 46 | -2.259 | 1.937 | 3.634 |
| ATOM | 434 | CB | MET | A | 46 | -2.166 | -0.088 | 1.379 |
| ATOM | 435 | CG | MET | A | 46 | -2.782 | -0.366 | 0.053 |
| ATOM | 436 | SD | MET | A | 46 | -3.076 | -2.108 | -0.118 |
| ATOM | 437 | CE | MET | A | 46 | -1.417 | -2.652 | -0.186 |
| ATOM | 438 | N | ILE | A | 47 | -1.827 | -0.016 | 4.586 |
| ATOM | 439 | H | ILE | A | 47 | -2.010 | -0.997 | 4.655 |
| ATOM | 440 | CA | ILE | A | 47 | -0.922 | 0.586 | 5.539 |
| ATOM | 441 | C | ILE | A | 47 | 0.233 | -0.372 | 5.654 |
| ATOM | 442 | O | ILE | A | 47 | 0.135 | -1.584 | 5.356 |
| ATOM | 443 | CB | ILE | A | 47 | -1.550 | 0.836 | 6.923 |
| ATOM | 444 | CG1 | ILE | A | 47 | -2.459 | -0.301 | 7.354 |
| ATOM | 445 | CG2 | ILE | A | 47 | -2.248 | 2.164 | 6.995 |
| ATOM | 446 | CD1 | ILE | A | 47 | -1.724 | -1.336 | 8.111 |
| ATOM | 447 | N | GLY | A | 48 | 1.420 | 0.089 | 6.043 |

FIG. 1 IH

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 448 | H | GLY | A | 48 | 1.509 | 1.040 | 6.339 |
| ATOM | 449 | CA | GLY | A | 48 | 2.584 | -0.753 | 6.048 |
| ATOM | 450 | C | GLY | A | 48 | 3.280 | -0.657 | 7.376 |
| ATOM | 451 | O | GLY | A | 48 | 3.050 | 0.190 | 8.265 |
| ATOM | 452 | N | GLY | A | 49 | 4.197 | -1.617 | 7.603 |
| ATOM | 453 | H | GLY | A | 49 | 4.375 | -2.308 | 6.902 |
| ATOM | 454 | CA | GLY | A | 49 | 4.936 | -1.684 | 8.828 |
| ATOM | 455 | C | GLY | A | 49 | 6.105 | -2.589 | 8.533 |
| ATOM | 456 | O | GLY | A | 49 | 6.482 | -2.807 | 7.370 |
| ATOM | 457 | N | ILE | A | 50 | 6.761 | -3.173 | 9.552 |
| ATOM | 458 | H | ILE | A | 50 | 6.552 | -2.908 | 10.493 |
| ATOM | 459 | CA | ILE | A | 50 | 7.772 | -4.184 | 9.344 |
| ATOM | 460 | C | ILE | A | 50 | 7.148 | -5.317 | 8.566 |
| ATOM | 461 | O | ILE | A | 50 | 5.981 | -5.734 | 8.772 |
| ATOM | 462 | CB | ILE | A | 50 | 8.258 | -4.686 | 10.722 |
| ATOM | 463 | CG1 | ILE | A | 50 | 9.257 | -3.714 | 11.382 |
| ATOM | 464 | CG2 | ILE | A | 50 | 8.813 | -6.134 | 10.693 |
| ATOM | 465 | CD1 | ILE | A | 50 | 10.580 | -3.498 | 10.628 |
| ATOM | 466 | N | GLY | A | 51 | 7.847 | -5.891 | 7.596 |
| ATOM | 467 | H | GLY | A | 51 | 8.772 | -5.569 | 7.395 |
| ATOM | 468 | CA | GLY | A | 51 | 7.265 | -6.966 | 6.850 |
| ATOM | 469 | C | GLY | A | 51 | 6.519 | -6.559 | 5.591 |
| ATOM | 470 | O | GLY | A | 51 | 6.430 | -7.318 | 4.634 |
| ATOM | 471 | N | GLY | A | 52 | 5.886 | -5.375 | 5.517 |
| ATOM | 472 | H | GLY | A | 52 | 5.990 | -4.710 | 6.257 |
| ATOM | 473 | CA | GLY | A | 52 | 5.108 | -5.227 | 4.320 |
| ATOM | 474 | C | GLY | A | 52 | 3.832 | -4.415 | 4.516 |
| ATOM | 475 | O | GLY | A | 52 | 3.654 | -3.624 | 5.467 |
| ATOM | 476 | N | PHE | A | 53 | 2.886 | -4.518 | 3.559 |
| ATOM | 477 | H | PHE | A | 53 | 3.013 | -5.161 | 2.804 |
| ATOM | 478 | CA | PHE | A | 53 | 1.653 | -3.720 | 3.566 |
| ATOM | 479 | C | PHE | A | 53 | 0.494 | -4.651 | 3.783 |
| ATOM | 480 | O | PHE | A | 53 | 0.448 | -5.816 | 3.336 |
| ATOM | 481 | CB | PHE | A | 53 | 1.424 | -3.022 | 2.221 |
| ATOM | 482 | CG | PHE | A | 53 | 2.363 | -1.896 | 2.008 |
| ATOM | 483 | CD1 | PHE | A | 53 | 3.615 | -2.135 | 1.447 |
| ATOM | 484 | CD2 | PHE | A | 53 | 2.011 | -0.608 | 2.414 |
| ATOM | 485 | CE1 | PHE | A | 53 | 4.514 | -1.087 | 1.275 |
| ATOM | 486 | CE2 | PHE | A | 53 | 2.925 | 0.446 | 2.237 |
| ATOM | 487 | CZ | PHE | A | 53 | 4.172 | 0.202 | 1.668 |
| ATOM | 488 | N | ILE | A | 54 | -0.554 | -4.173 | 4.439 |
| ATOM | 489 | H | ILE | A | 54 | -0.491 | -3.285 | 4.895 |
| ATOM | 490 | CA | ILE | A | 54 | -1.789 | -4.911 | 4.509 |
| ATOM | 491 | C | ILE | A | 54 | -2.903 | -3.995 | 4.033 |
| ATOM | 492 | O | ILE | A | 54 | -2.751 | -2.770 | 3.855 |
| ATOM | 493 | CB | ILE | A | 54 | -2.034 | -5.535 | 5.904 |
| ATOM | 494 | CG1 | ILE | A | 54 | -2.343 | -4.481 | 6.988 |
| ATOM | 495 | CG2 | ILE | A | 54 | -0.799 | -6.318 | 6.314 |
| ATOM | 496 | CD1 | ILE | A | 54 | -3.010 | -5.089 | 8.246 |
| ATOM | 497 | N | LYS | A | 55 | -4.029 | -4.577 | 3.560 |
| ATOM | 498 | H | LYS | A | 55 | -4.084 | -5.574 | 3.501 |
| ATOM | 499 | CA | LYS | A | 55 | -5.177 | -3.798 | 3.129 |
| ATOM | 500 | C | LYS | A | 55 | -6.115 | -3.726 | 4.300 |
| ATOM | 501 | O | LYS | A | 55 | -6.422 | -4.707 | 5.023 |
| ATOM | 502 | CB | LYS | A | 55 | -5.928 | -4.461 | 1.938 |
| ATOM | 503 | CG | LYS | A | 55 | -6.853 | -3.547 | 1.106 |

FIG. 11I

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 504 | CD | LYS | A | 55 | -8.267 | -3.332 | 1.714 |
| ATOM | 505 | CE | LYS | A | 55 | -9.303 | -4.392 | 1.301 |
| ATOM | 506 | NZ | LYS | A | 55 | -10.521 | -4.453 | 2.192 |
| ATOM | 507 | 1HZ | LYS | A | 55 | -11.142 | -5.162 | 1.859 |
| ATOM | 508 | 3HZ | LYS | A | 55 | -10.987 | -3.569 | 2.180 |
| ATOM | 509 | 2HZ | LYS | A | 55 | -10.240 | -4.669 | 3.127 |
| ATOM | 510 | N | VAL | A | 56 | -6.599 | -2.509 | 4.619 |
| ATOM | 511 | H | VAL | A | 56 | -6.337 | -1.713 | 4.073 |
| ATOM | 512 | CA | VAL | A | 56 | -7.494 | -2.311 | 5.735 |
| ATOM | 513 | C | VAL | A | 56 | -8.711 | -1.584 | 5.236 |
| ATOM | 514 | O | VAL | A | 56 | -8.767 | -1.029 | 4.114 |
| ATOM | 515 | CB | VAL | A | 56 | -6.759 | -1.475 | 6.812 |
| ATOM | 516 | CG1 | VAL | A | 56 | -5.569 | -2.209 | 7.385 |
| ATOM | 517 | CG2 | VAL | A | 56 | -6.287 | -0.108 | 6.268 |
| ATOM | 518 | N | ARG | A | 57 | -9.784 | -1.539 | 6.005 |
| ATOM | 519 | H | ARG | A | 57 | -9.835 | -2.117 | 6.819 |
| ATOM | 520 | CA | ARG | A | 57 | -10.855 | -0.648 | 5.638 |
| ATOM | 521 | C | ARG | A | 57 | -10.738 | 0.534 | 6.554 |
| ATOM | 522 | O | ARG | A | 57 | -10.558 | 0.449 | 7.789 |
| ATOM | 523 | CB | ARG | A | 57 | -12.219 | -1.271 | 5.835 |
| ATOM | 524 | CG | ARG | A | 57 | -12.480 | -2.452 | 4.952 |
| ATOM | 525 | CD | ARG | A | 57 | -13.834 | -3.051 | 5.195 |
| ATOM | 526 | NE | ARG | A | 57 | -14.122 | -4.137 | 4.270 |
| ATOM | 527 | HE | ARG | A | 57 | -13.442 | -4.347 | 3.568 |
| ATOM | 528 | CZ | ARG | A | 57 | -15.243 | -4.851 | 4.324 |
| ATOM | 529 | NH1 | ARG | A | 57 | -16.175 | -4.624 | 5.243 |
| ATOM | 530 | 2HH1 | ARG | A | 57 | -16.044 | -3.899 | 5.920 |
| ATOM | 531 | 1HH1 | ARG | A | 57 | -17.008 | -5.178 | 5.258 |
| ATOM | 532 | NH2 | ARG | A | 57 | -15.433 | -5.822 | 3.434 |
| ATOM | 533 | 1HH2 | ARG | A | 57 | -16.270 | -6.368 | 3.461 |
| ATOM | 534 | 2HH2 | ARG | A | 57 | -14.738 | -6.006 | 2.738 |
| ATOM | 535 | N | GLN | A | 58 | -10.881 | 1.741 | 6.036 |
| ATOM | 536 | H | GLN | A | 58 | -11.030 | 1.844 | 5.053 |
| ATOM | 537 | CA | GLN | A | 58 | -10.830 | 2.922 | 6.839 |
| ATOM | 538 | C | GLN | A | 58 | -12.231 | 3.342 | 7.205 |
| ATOM | 539 | O | GLN | A | 58 | -13.106 | 3.608 | 6.359 |
| ATOM | 540 | CB | GLN | A | 58 | -10.208 | 4.038 | 6.030 |
| ATOM | 541 | CG | GLN | A | 58 | -10.055 | 5.293 | 6.817 |
| ATOM | 542 | CD | GLN | A | 58 | -9.632 | 6.411 | 5.927 |
| ATOM | 543 | OE1 | GLN | A | 58 | -10.379 | 7.334 | 5.662 |
| ATOM | 544 | NE2 | GLN | A | 58 | -8.412 | 6.303 | 5.437 |
| ATOM | 545 | 1HE2 | GLN | A | 58 | -8.047 | 7.009 | 4.830 |
| ATOM | 546 | 2HE2 | GLN | A | 58 | -7.843 | 5.514 | 5.668 |
| ATOM | 547 | N | TYR | A | 59 | -12.527 | 3.516 | 8.509 |
| ATOM | 548 | H | TYR | A | 59 | -11.877 | 3.219 | 9.209 |
| ATOM | 549 | CA | TYR | A | 59 | -13.769 | 4.125 | 8.933 |
| ATOM | 550 | C | TYR | A | 59 | -13.411 | 5.452 | 9.565 |
| ATOM | 551 | O | TYR | A | 59 | -12.416 | 5.592 | 10.310 |
| ATOM | 552 | CB | TYR | A | 59 | -14.517 | 3.252 | 9.957 |
| ATOM | 553 | CG | TYR | A | 59 | -14.287 | 1.770 | 9.723 |
| ATOM | 554 | CD1 | TYR | A | 59 | -13.007 | 1.269 | 9.457 |
| ATOM | 555 | CD2 | TYR | A | 59 | -15.346 | 0.865 | 9.766 |
| ATOM | 556 | CE1 | TYR | A | 59 | -12.797 | -0.092 | 9.240 |
| ATOM | 557 | CE2 | TYR | A | 59 | -15.148 | -0.494 | 9.551 |
| ATOM | 558 | CZ | TYR | A | 59 | -13.873 | -0.972 | 9.287 |
| ATOM | 559 | OH | TYR | A | 59 | -13.721 | -2.311 | 9.079 |

FIG. 11J

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 560 | HH | TYR | A | 59 | -14.606 | -2.771 | 9.154 |
| ATOM | 561 | N | ASP | A | 60 | -14.151 | 6.542 | 9.300 |
| ATOM | 562 | H | ASP | A | 60 | -14.954 | 6.464 | 8.709 |
| ATOM | 563 | CA | ASP | A | 60 | -13.822 | 7.836 | 9.846 |
| ATOM | 564 | C | ASP | A | 60 | -14.782 | 8.226 | 10.947 |
| ATOM | 565 | O | ASP | A | 60 | -15.941 | 7.765 | 11.053 |
| ATOM | 566 | CB | ASP | A | 60 | -13.861 | 8.942 | 8.769 |
| ATOM | 567 | CG | ASP | A | 60 | -12.735 | 8.830 | 7.725 |
| ATOM | 568 | OD1 | ASP | A | 60 | -11.545 | 8.874 | 8.075 |
| ATOM | 569 | OD2 | ASP | A | 60 | -13.060 | 8.702 | 6.544 |
| ATOM | 570 | N | GLN | A | 61 | -14.339 | 9.154 | 11.833 |
| ATOM | 571 | H | GLN | A | 61 | -13.385 | 9.451 | 11.804 |
| ATOM | 572 | CA | GLN | A | 61 | -15.151 | 9.804 | 12.885 |
| ATOM | 573 | C | GLN | A | 61 | -15.839 | 8.803 | 13.802 |
| ATOM | 574 | O | GLN | A | 61 | -17.008 | 8.893 | 14.229 |
| ATOM | 575 | CB | GLN | A | 61 | -16.097 | 10.908 | 12.338 |
| ATOM | 576 | CG | GLN | A | 61 | -16.239 | 12.133 | 13.262 |
| ATOM | 577 | CD | GLN | A | 61 | -16.910 | 13.366 | 12.629 |
| ATOM | 578 | OE1 | GLN | A | 61 | -16.509 | 13.854 | 11.586 |
| ATOM | 579 | NE2 | GLN | A | 61 | -17.937 | 13.887 | 13.292 |
| ATOM | 580 | 1HE2 | GLN | A | 61 | -18.416 | 14.689 | 12.934 |
| ATOM | 581 | 2HE2 | GLN | A | 61 | -18.239 | 13.482 | 14.155 |
| ATOM | 582 | N | ILE | A | 62 | -15.060 | 7.760 | 14.175 |
| ATOM | 583 | H | ILE | A | 62 | -14.111 | 7.714 | 13.862 |
| ATOM | 584 | CA | ILE | A | 62 | -15.557 | 6.705 | 15.015 |
| ATOM | 585 | C | ILE | A | 62 | -15.251 | 7.057 | 16.447 |
| ATOM | 586 | O | ILE | A | 62 | -14.198 | 7.613 | 16.837 |
| ATOM | 587 | CB | ILE | A | 62 | -14.829 | 5.397 | 14.653 |
| ATOM | 588 | CG1 | ILE | A | 62 | -15.253 | 4.966 | 13.258 |
| ATOM | 589 | CG2 | ILE | A | 62 | -15.106 | 4.271 | 15.675 |
| ATOM | 590 | CD1 | ILE | A | 62 | -16.779 | 4.788 | 13.116 |
| ATOM | 591 | N | LEU | A | 63 | -16.242 | 6.807 | 17.320 |
| ATOM | 592 | H | LEU | A | 63 | -17.089 | 6.383 | 17.000 |
| ATOM | 593 | CA | LEU | A | 63 | -16.127 | 7.131 | 18.719 |
| ATOM | 594 | C | LEU | A | 63 | -15.518 | 5.942 | 19.425 |
| ATOM | 595 | O | LEU | A | 63 | -15.869 | 4.753 | 19.269 |
| ATOM | 596 | CB | LEU | A | 63 | -17.512 | 7.428 | 19.282 |
| ATOM | 597 | CG | LEU | A | 63 | -17.660 | 7.598 | 20.813 |
| ATOM | 598 | CD1 | LEU | A | 63 | -16.711 | 8.632 | 21.404 |
| ATOM | 599 | CD2 | LEU | A | 63 | -19.089 | 7.963 | 21.201 |
| ATOM | 600 | N | ILE | A | 64 | -14.511 | 6.211 | 20.219 |
| ATOM | 601 | H | ILE | A | 64 | -14.185 | 7.153 | 20.305 |
| ATOM | 602 | CA | ILE | A | 64 | -13.862 | 5.178 | 20.972 |
| ATOM | 603 | C | ILE | A | 64 | -13.529 | 5.744 | 22.325 |
| ATOM | 604 | O | ILE | A | 64 | -13.396 | 6.959 | 22.602 |
| ATOM | 605 | CB | ILE | A | 64 | -12.618 | 4.716 | 20.231 |
| ATOM | 606 | CG1 | ILE | A | 64 | -11.925 | 3.573 | 20.949 |
| ATOM | 607 | CG2 | ILE | A | 64 | -11.690 | 5.865 | 19.950 |
| ATOM | 608 | CD1 | ILE | A | 64 | -10.905 | 2.888 | 20.062 |
| ATOM | 609 | N | GLU | A | 65 | -13.396 | 4.815 | 23.294 |
| ATOM | 610 | H | GLU | A | 65 | -13.443 | 3.844 | 23.059 |
| ATOM | 611 | CA | GLU | A | 65 | -13.186 | 5.174 | 24.670 |
| ATOM | 612 | C | GLU | A | 65 | -12.024 | 4.360 | 25.165 |
| ATOM | 613 | O | GLU | A | 65 | -11.943 | 3.112 | 25.056 |
| ATOM | 614 | CB | GLU | A | 65 | -14.459 | 4.823 | 25.405 |
| ATOM | 615 | CG | GLU | A | 65 | -14.739 | 5.610 | 26.646 |

FIG. 11K

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 616 | CD | GLU | A | 65 | -16.131 | 5.353 | 27.115 |
| ATOM | 617 | OE1 | GLU | A | 65 | -17.090 | 5.785 | 26.413 |
| ATOM | 618 | OE2 | GLU | A | 65 | -16.269 | 4.708 | 28.163 |
| ATOM | 619 | N | ILE | A | 66 | -10.971 | 5.008 | 25.610 |
| ATOM | 620 | H | ILE | A | 66 | -11.009 | 6.002 | 25.717 |
| ATOM | 621 | CA | ILE | A | 66 | -9.762 | 4.317 | 25.947 |
| ATOM | 622 | C | ILE | A | 66 | -9.571 | 4.586 | 27.413 |
| ATOM | 623 | O | ILE | A | 66 | -9.422 | 5.732 | 27.880 |
| ATOM | 624 | CB | ILE | A | 66 | -8.600 | 4.907 | 25.126 |
| ATOM | 625 | CG1 | ILE | A | 66 | -8.838 | 4.669 | 23.633 |
| ATOM | 626 | CG2 | ILE | A | 66 | -7.231 | 4.326 | 25.554 |
| ATOM | 627 | CD1 | ILE | A | 66 | -8.951 | 5.982 | 22.856 |
| ATOM | 628 | N | CYS | A | 67 | -9.776 | 3.567 | 28.261 |
| ATOM | 629 | H | CYS | A | 67 | -9.989 | 2.659 | 27.902 |
| ATOM | 630 | CA | CYS | A | 67 | -9.698 | 3.740 | 29.687 |
| ATOM | 631 | C | CYS | A | 67 | -10.673 | 4.871 | 30.088 |
| ATOM | 632 | O | CYS | A | 67 | -10.393 | 5.716 | 30.958 |
| ATOM | 633 | CB | CYS | A | 67 | -8.251 | 4.003 | 30.156 |
| ATOM | 634 | SG | CYS | A | 67 | -7.170 | 2.529 | 30.217 |
| ATOM | 635 | N | GLY | A | 68 | -11.877 | 4.947 | 29.499 |
| ATOM | 636 | H | GLY | A | 68 | -12.125 | 4.286 | 28.791 |
| ATOM | 637 | CA | GLY | A | 68 | -12.788 | 5.984 | 29.903 |
| ATOM | 638 | C | GLY | A | 68 | -12.581 | 7.322 | 29.241 |
| ATOM | 639 | O | GLY | A | 68 | -13.404 | 8.253 | 29.376 |
| ATOM | 640 | N | HIS | A | 69 | -11.504 | 7.545 | 28.471 |
| ATOM | 641 | H | HIS | A | 69 | -10.817 | 6.827 | 28.360 |
| ATOM | 642 | CA | HIS | A | 69 | -11.305 | 8.800 | 27.793 |
| ATOM | 643 | C | HIS | A | 69 | -11.838 | 8.679 | 26.399 |
| ATOM | 644 | O | HIS | A | 69 | -11.516 | 7.742 | 25.630 |
| ATOM | 645 | CB | HIS | A | 69 | -9.831 | 9.128 | 27.724 |
| ATOM | 646 | CG | HIS | A | 69 | -9.276 | 9.286 | 29.081 |
| ATOM | 647 | ND1 | HIS | A | 69 | -9.317 | 10.484 | 29.778 |
| ATOM | 648 | HD1 | HIS | A | 69 | -9.688 | 11.347 | 29.436 |
| ATOM | 649 | CD2 | HIS | A | 69 | -8.723 | 8.352 | 29.912 |
| ATOM | 650 | CE1 | HIS | A | 69 | -8.783 | 10.254 | 30.947 |
| ATOM | 651 | NE2 | HIS | A | 69 | -8.405 | 8.990 | 31.091 |
| ATOM | 652 | N | LYS | A | 70 | -12.768 | 9.561 | 25.973 |
| ATOM | 653 | H | LYS | A | 70 | -13.084 | 10.284 | 26.588 |
| ATOM | 654 | CA | LYS | A | 70 | -13.325 | 9.492 | 24.646 |
| ATOM | 655 | C | LYS | A | 70 | -12.346 | 10.074 | 23.653 |
| ATOM | 656 | O | LYS | A | 70 | -11.587 | 11.055 | 23.864 |
| ATOM | 657 | CB | LYS | A | 70 | -14.645 | 10.285 | 24.536 |
| ATOM | 658 | CG | LYS | A | 70 | -15.837 | 9.703 | 25.330 |
| ATOM | 659 | CD | LYS | A | 70 | -17.105 | 10.593 | 25.286 |
| ATOM | 660 | CE | LYS | A | 70 | -18.293 | 10.011 | 26.092 |
| ATOM | 661 | NZ | LYS | A | 70 | -18.802 | 8.702 | 25.608 |
| ATOM | 662 | 1HZ | LYS | A | 70 | -19.563 | 8.406 | 26.185 |
| ATOM | 663 | 3HZ | LYS | A | 70 | -18.069 | 8.023 | 25.650 |
| ATOM | 664 | 2HZ | LYS | A | 70 | -19.116 | 8.795 | 24.663 |
| ATOM | 665 | N | ALA | A | 71 | -12.323 | 9.485 | 22.446 |
| ATOM | 666 | H | ALA | A | 71 | -12.813 | 8.625 | 22.305 |
| ATOM | 667 | CA | ALA | A | 71 | -11.616 | 10.044 | 21.333 |
| ATOM | 668 | C | ALA | A | 71 | -12.529 | 9.795 | 20.171 |
| ATOM | 669 | O | ALA | A | 71 | -13.351 | 8.850 | 20.146 |
| ATOM | 670 | CB | ALA | A | 71 | -10.292 | 9.358 | 21.143 |
| ATOM | 671 | N | ILE | A | 72 | -12.559 | 10.685 | 19.149 |

FIG. 1 IL

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 672 | H | ILE | A | 72 | -12.006 | 11.517 | 19.200 |
| ATOM | 673 | CA | ILE | A | 72 | -13.376 | 10.474 | 17.963 |
| ATOM | 674 | C | ILE | A | 72 | -12.480 | 10.662 | 16.771 |
| ATOM | 675 | O | ILE | A | 72 | -11.858 | 11.720 | 16.550 |
| ATOM | 676 | CB | ILE | A | 72 | -14.541 | 11.464 | 17.882 |
| ATOM | 677 | CG1 | ILE | A | 72 | -15.306 | 11.455 | 19.196 |
| ATOM | 678 | CG2 | ILE | A | 72 | -15.429 | 11.203 | 16.651 |
| ATOM | 679 | CD1 | ILE | A | 72 | -16.446 | 12.415 | 19.176 |
| ATOM | 680 | N | GLY | A | 73 | -12.252 | 9.633 | 15.958 |
| ATOM | 681 | H | GLY | A | 73 | -12.778 | 8.789 | 16.067 |
| ATOM | 682 | CA | GLY | A | 73 | -11.253 | 9.755 | 14.938 |
| ATOM | 683 | C | GLY | A | 73 | -11.283 | 8.554 | 14.034 |
| ATOM | 684 | O | GLY | A | 73 | -12.211 | 7.706 | 14.006 |
| ATOM | 685 | N | THR | A | 74 | -10.247 | 8.428 | 13.182 |
| ATOM | 686 | H | THR | A | 74 | -9.471 | 9.055 | 13.250 |
| ATOM | 687 | CA | THR | A | 74 | -10.201 | 7.416 | 12.158 |
| ATOM | 688 | C | THR | A | 74 | -9.674 | 6.134 | 12.760 |
| ATOM | 689 | O | THR | A | 74 | -8.670 | 6.034 | 13.497 |
| ATOM | 690 | CB | THR | A | 74 | -9.298 | 7.895 | 11.048 |
| ATOM | 691 | OG1 | THR | A | 74 | -9.910 | 9.019 | 10.441 |
| ATOM | 692 | HG1 | THR | A | 74 | -9.335 | 9.362 | 9.698 |
| ATOM | 693 | CG2 | THR | A | 74 | -9.088 | 6.823 | 9.946 |
| ATOM | 694 | N | VAL | A | 75 | -10.318 | 5.027 | 12.327 |
| ATOM | 695 | H | VAL | A | 75 | -11.066 | 5.114 | 11.669 |
| ATOM | 696 | CA | VAL | A | 75 | -9.968 | 3.717 | 12.778 |
| ATOM | 697 | C | VAL | A | 75 | -9.906 | 2.843 | 11.551 |
| ATOM | 698 | O | VAL | A | 75 | -10.803 | 2.807 | 10.681 |
| ATOM | 699 | CB | VAL | A | 75 | -11.044 | 3.250 | 13.737 |
| ATOM | 700 | CG1 | VAL | A | 75 | -11.021 | 1.721 | 13.943 |
| ATOM | 701 | CG2 | VAL | A | 75 | -10.915 | 4.019 | 15.034 |
| ATOM | 702 | N | LEU | A | 76 | -8.768 | 2.139 | 11.366 |
| ATOM | 703 | H | LEU | A | 76 | -8.002 | 2.260 | 11.998 |
| ATOM | 704 | CA | LEU | A | 76 | -8.566 | 1.183 | 10.276 |
| ATOM | 705 | C | LEU | A | 76 | -8.848 | -0.211 | 10.808 |
| ATOM | 706 | O | LEU | A | 76 | -8.514 | -0.582 | 11.958 |
| ATOM | 707 | CB | LEU | A | 76 | -7.103 | 1.270 | 9.798 |
| ATOM | 708 | CG | LEU | A | 76 | -6.608 | 2.684 | 9.443 |
| ATOM | 709 | CD1 | LEU | A | 76 | -5.151 | 2.645 | 9.087 |
| ATOM | 710 | CD2 | LEU | A | 76 | -7.396 | 3.302 | 8.296 |
| ATOM | 711 | N | VAL | A | 77 | -9.569 | -1.062 | 10.042 |
| ATOM | 712 | H | VAL | A | 77 | -9.894 | -0.766 | 9.144 |
| ATOM | 713 | CA | VAL | A | 77 | -9.899 | -2.428 | 10.485 |
| ATOM | 714 | C | VAL | A | 77 | -9.298 | -3.412 | 9.482 |
| ATOM | 715 | O | VAL | A | 77 | -9.450 | -3.300 | 8.253 |
| ATOM | 716 | CB | VAL | A | 77 | -11.436 | -2.592 | 10.506 |
| ATOM | 717 | CG1 | VAL | A | 77 | -11.830 | -4.021 | 10.682 |
| ATOM | 718 | CG2 | VAL | A | 77 | -12.072 | -1.765 | 11.634 |
| ATOM | 719 | N | GLY | A | 78 | -8.560 | -4.402 | 9.928 |
| ATOM | 720 | H | GLY | A | 78 | -8.445 | -4.530 | 10.913 |
| ATOM | 721 | CA | GLY | A | 78 | -7.930 | -5.285 | 8.987 |
| ATOM | 722 | C | GLY | A | 78 | -7.228 | -6.380 | 9.732 |
| ATOM | 723 | O | GLY | A | 78 | -7.292 | -6.524 | 10.970 |
| ATOM | 724 | N | PRO | A | 79 | -6.512 | -7.271 | 9.003 |
| ATOM | 725 | CA | PRO | A | 79 | -5.880 | -8.467 | 9.602 |
| ATOM | 726 | C | PRO | A | 79 | -4.599 | -8.107 | 10.340 |
| ATOM | 727 | O | PRO | A | 79 | -3.449 | -8.489 | 10.032 |

FIG. 1 IM

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 728 | CB | PRO | A | 79 | -5.613 | -9.379 | 8.400 |
| ATOM | 729 | CG | PRO | A | 79 | -5.529 | -8.416 | 7.210 |
| ATOM | 730 | CD | PRO | A | 79 | -6.415 | -7.225 | 7.537 |
| ATOM | 731 | N | THR | A | 80 | -4.759 | -7.304 | 11.408 |
| ATOM | 732 | H | THR | A | 80 | -5.664 | -6.935 | 11.619 |
| ATOM | 733 | CA | THR | A | 80 | -3.658 | -6.957 | 12.263 |
| ATOM | 734 | C | THR | A | 80 | -3.490 | -8.075 | 13.308 |
| ATOM | 735 | O | THR | A | 80 | -4.447 | -8.642 | 13.857 |
| ATOM | 736 | CB | THR | A | 80 | -3.868 | -5.572 | 12.927 |
| ATOM | 737 | OG1 | THR | A | 80 | -2.770 | -5.303 | 13.787 |
| ATOM | 738 | HG1 | THR | A | 80 | -2.889 | -4.412 | 14.225 |
| ATOM | 739 | CG2 | THR | A | 80 | -5.210 | -5.464 | 13.678 |
| ATOM | 740 | N | PRO | A | 81 | -2.243 | -8.496 | 13.589 |
| ATOM | 741 | CA | PRO | A | 81 | -1.986 | -9.476 | 14.660 |
| ATOM | 742 | C | PRO | A | 81 | -2.499 | -8.952 | 16.001 |
| ATOM | 743 | O | PRO | A | 81 | -2.944 | -9.720 | 16.866 |
| ATOM | 744 | CB | PRO | A | 81 | -0.444 | -9.549 | 14.732 |
| ATOM | 745 | CG | PRO | A | 81 | 0.069 | -8.951 | 13.429 |
| ATOM | 746 | CD | PRO | A | 81 | -1.029 | -8.105 | 12.842 |
| ATOM | 747 | N | VAL | A | 82 | -2.474 | -7.621 | 16.276 |
| ATOM | 748 | H | VAL | A | 82 | -2.180 | -6.975 | 15.571 |
| ATOM | 749 | CA | VAL | A | 82 | -2.869 | -7.091 | 17.591 |
| ATOM | 750 | C | VAL | A | 82 | -3.605 | -5.761 | 17.379 |
| ATOM | 751 | O | VAL | A | 82 | -3.349 | -5.004 | 16.429 |
| ATOM | 752 | CB | VAL | A | 82 | -1.595 | -6.858 | 18.443 |
| ATOM | 753 | CG1 | VAL | A | 82 | -0.650 | -5.824 | 17.803 |
| ATOM | 754 | CG2 | VAL | A | 82 | -1.907 | -6.418 | 19.890 |
| ATOM | 755 | N | ASN | A | 83 | -4.548 | -5.371 | 18.260 |
| ATOM | 756 | H | ASN | A | 83 | -4.810 | -5.981 | 19.007 |
| ATOM | 757 | CA | ASN | A | 83 | -5.181 | -4.067 | 18.123 |
| ATOM | 758 | C | ASN | A | 83 | -4.195 | -3.019 | 18.565 |
| ATOM | 759 | O | ASN | A | 83 | -3.605 | -3.064 | 19.665 |
| ATOM | 760 | CB | ASN | A | 83 | -6.436 | -3.942 | 18.982 |
| ATOM | 761 | CG | ASN | A | 83 | -7.502 | -4.930 | 18.631 |
| ATOM | 762 | OD1 | ASN | A | 83 | -7.899 | -5.049 | 17.488 |
| ATOM | 763 | ND2 | ASN | A | 83 | -7.980 | -5.662 | 19.628 |
| ATOM | 764 | 2HD2 | ASN | A | 83 | -8.695 | -6.341 | 19.459 |
| ATOM | 765 | 1HD2 | ASN | A | 83 | -7.630 | -5.541 | 20.557 |
| ATOM | 766 | N | ILE | A | 84 | -4.007 | -1.951 | 17.770 |
| ATOM | 767 | H | ILE | A | 84 | -4.583 | -1.827 | 16.962 |
| ATOM | 768 | CA | ILE | A | 84 | -2.993 | -0.954 | 18.032 |
| ATOM | 769 | C | ILE | A | 84 | -3.679 | 0.387 | 18.114 |
| ATOM | 770 | O | ILE | A | 84 | -4.460 | 0.797 | 17.240 |
| ATOM | 771 | CB | ILE | A | 84 | -2.021 | -0.922 | 16.833 |
| ATOM | 772 | CG1 | ILE | A | 84 | -1.162 | -2.150 | 16.859 |
| ATOM | 773 | CG2 | ILE | A | 84 | -1.219 | 0.387 | 16.747 |
| ATOM | 774 | CD1 | ILE | A | 84 | -0.375 | -2.360 | 15.579 |
| ATOM | 775 | N | ILE | A | 85 | -3.471 | 1.155 | 19.203 |
| ATOM | 776 | H | ILE | A | 85 | -2.972 | 0.781 | 19.985 |
| ATOM | 777 | CA | ILE | A | 85 | -3.951 | 2.518 | 19.281 |
| ATOM | 778 | C | ILE | A | 85 | -2.784 | 3.425 | 18.949 |
| ATOM | 779 | O | ILE | A | 85 | -1.767 | 3.515 | 19.663 |
| ATOM | 780 | CB | ILE | A | 85 | -4.522 | 2.825 | 20.676 |
| ATOM | 781 | CG1 | ILE | A | 85 | -5.673 | 1.865 | 21.050 |
| ATOM | 782 | CG2 | ILE | A | 85 | -5.000 | 4.274 | 20.716 |
| ATOM | 783 | CD1 | ILE | A | 85 | -6.828 | 1.808 | 20.059 |

FIG. 1 IN

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 784 | N | GLY | A | 86 | -2.820 | 4.123 | 17.792 |
| ATOM | 785 | H | GLY | A | 86 | -3.637 | 4.087 | 17.217 |
| ATOM | 786 | CA | GLY | A | 86 | -1.690 | 4.936 | 17.351 |
| ATOM | 787 | C | GLY | A | 86 | -1.831 | 6.393 | 17.704 |
| ATOM | 788 | O | GLY | A | 86 | -2.760 | 6.864 | 18.390 |
| ATOM | 789 | N | ARG | A | 87 | -0.881 | 7.229 | 17.230 |
| ATOM | 790 | H | ARG | A | 87 | -0.204 | 6.890 | 16.577 |
| ATOM | 791 | CA | ARG | A | 87 | -0.810 | 8.623 | 17.643 |
| ATOM | 792 | C | ARG | A | 87 | -2.027 | 9.445 | 17.277 |
| ATOM | 793 | O | ARG | A | 87 | -2.365 | 10.430 | 17.963 |
| ATOM | 794 | CB | ARG | A | 87 | 0.450 | 9.275 | 17.057 |
| ATOM | 795 | CG | ARG | A | 87 | 1.735 | 8.496 | 17.205 |
| ATOM | 796 | CD | ARG | A | 87 | 2.762 | 8.916 | 16.207 |
| ATOM | 797 | NE | ARG | A | 87 | 3.875 | 7.961 | 16.117 |
| ATOM | 798 | HE | ARG | A | 87 | 4.035 | 7.353 | 16.895 |
| ATOM | 799 | CZ | ARG | A | 87 | 4.660 | 7.893 | 15.035 |
| ATOM | 800 | NH1 | ARG | A | 87 | 4.463 | 8.675 | 13.975 |
| ATOM | 801 | 2HH1 | ARG | A | 87 | 3.712 | 9.335 | 13.974 |
| ATOM | 802 | 1HH1 | ARG | A | 87 | 5.066 | 8.602 | 13.181 |
| ATOM | 803 | NH2 | ARG | A | 87 | 5.656 | 7.019 | 15.023 |
| ATOM | 804 | 1HH2 | ARG | A | 87 | 6.254 | 6.953 | 14.224 |
| ATOM | 805 | 2HH2 | ARG | A | 87 | 5.810 | 6.426 | 15.813 |
| ATOM | 806 | N | ASN | A | 88 | -2.780 | 9.120 | 16.214 |
| ATOM | 807 | H | ASN | A | 88 | -2.504 | 8.361 | 15.625 |
| ATOM | 808 | CA | ASN | A | 88 | -4.015 | 9.860 | 15.890 |
| ATOM | 809 | C | ASN | A | 88 | -4.963 | 9.921 | 17.069 |
| ATOM | 810 | O | ASN | A | 88 | -5.613 | 10.954 | 17.345 |
| ATOM | 811 | CB | ASN | A | 88 | -4.712 | 9.315 | 14.617 |
| ATOM | 812 | CG | ASN | A | 88 | -5.475 | 8.001 | 14.827 |
| ATOM | 813 | OD1 | ASN | A | 88 | -4.922 | 6.996 | 15.245 |
| ATOM | 814 | ND2 | ASN | A | 88 | -6.758 | 7.998 | 14.506 |
| ATOM | 815 | 2HD2 | ASN | A | 88 | -7.306 | 7.169 | 14.622 |
| ATOM | 816 | 1HD2 | ASN | A | 88 | -7.190 | 8.824 | 14.145 |
| ATOM | 817 | N | LEU | A | 89 | -5.130 | 8.847 | 17.848 |
| ATOM | 818 | H | LEU | A | 89 | -4.637 | 8.002 | 17.640 |
| ATOM | 819 | CA | LEU | A | 89 | -6.024 | 8.865 | 19.013 |
| ATOM | 820 | C | LEU | A | 89 | -5.275 | 9.091 | 20.309 |
| ATOM | 821 | O | LEU | A | 89 | -5.834 | 9.632 | 21.283 |
| ATOM | 822 | CB | LEU | A | 89 | -6.840 | 7.592 | 19.140 |
| ATOM | 823 | CG | LEU | A | 89 | -7.759 | 7.355 | 17.957 |
| ATOM | 824 | CD1 | LEU | A | 89 | -8.369 | 5.980 | 18.088 |
| ATOM | 825 | CD2 | LEU | A | 89 | -8.817 | 8.457 | 17.801 |
| ATOM | 826 | N | LEU | A | 90 | -3.983 | 8.745 | 20.428 |
| ATOM | 827 | H | LEU | A | 90 | -3.525 | 8.274 | 19.674 |
| ATOM | 828 | CA | LEU | A | 90 | -3.242 | 9.057 | 21.664 |
| ATOM | 829 | C | LEU | A | 90 | -3.155 | 10.555 | 21.932 |
| ATOM | 830 | O | LEU | A | 90 | -3.202 | 11.020 | 23.092 |
| ATOM | 831 | CB | LEU | A | 90 | -1.817 | 8.453 | 21.661 |
| ATOM | 832 | CG | LEU | A | 90 | -1.766 | 6.914 | 21.587 |
| ATOM | 833 | CD1 | LEU | A | 90 | -0.343 | 6.494 | 21.396 |
| ATOM | 834 | CD2 | LEU | A | 90 | -2.339 | 6.230 | 22.812 |
| ATOM | 835 | N | THR | A | 91 | -3.031 | 11.407 | 20.926 |
| ATOM | 836 | H | THR | A | 91 | -2.982 | 11.063 | 19.988 |
| ATOM | 837 | CA | THR | A | 91 | -2.964 | 12.834 | 21.155 |
| ATOM | 838 | C | THR | A | 91 | -4.309 | 13.331 | 21.635 |
| ATOM | 839 | O | THR | A | 91 | -4.422 | 14.315 | 22.398 |

FIG. 110

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 840 | CB | THR | A | 91 | -2.555 | 13.543 | 19.848 |
| ATOM | 841 | OG1 | THR | A | 91 | -3.459 | 13.214 | 18.802 |
| ATOM | 842 | HG1 | THR | A | 91 | -3.188 | 13.677 | 17.958 |
| ATOM | 843 | CG2 | THR | A | 91 | -1.153 | 13.122 | 19.395 |
| ATOM | 844 | N | GLN | A | 92 | -5.435 | 12.704 | 21.258 |
| ATOM | 845 | H | GLN | A | 92 | -5.379 | 11.892 | 20.677 |
| ATOM | 846 | CA | GLN | A | 92 | -6.763 | 13.186 | 21.682 |
| ATOM | 847 | C | GLN | A | 92 | -6.942 | 12.975 | 23.153 |
| ATOM | 848 | O | GLN | A | 92 | -7.554 | 13.797 | 23.871 |
| ATOM | 849 | CB | GLN | A | 92 | -7.890 | 12.479 | 20.964 |
| ATOM | 850 | CG | GLN | A | 92 | -7.937 | 12.862 | 19.517 |
| ATOM | 851 | CD | GLN | A | 92 | -9.251 | 12.515 | 18.886 |
| ATOM | 852 | OE1 | GLN | A | 92 | -10.270 | 12.424 | 19.546 |
| ATOM | 853 | NE2 | GLN | A | 92 | -9.202 | 12.323 | 17.588 |
| ATOM | 854 | 1HE2 | GLN | A | 92 | -10.031 | 12.087 | 17.080 |
| ATOM | 855 | 2HE2 | GLN | A | 92 | -8.336 | 12.411 | 17.097 |
| ATOM | 856 | N | ILE | A | 93 | -6.472 | 11.846 | 23.721 |
| ATOM | 857 | H | ILE | A | 93 | -6.014 | 11.160 | 23.155 |
| ATOM | 858 | CA | ILE | A | 93 | -6.608 | 11.578 | 25.165 |
| ATOM | 859 | C | ILE | A | 93 | -5.472 | 12.189 | 25.948 |
| ATOM | 860 | O | ILE | A | 93 | -5.342 | 12.031 | 27.171 |
| ATOM | 861 | CB | ILE | A | 93 | -6.820 | 10.073 | 25.484 |
| ATOM | 862 | CG1 | ILE | A | 93 | -5.536 | 9.221 | 25.286 |
| ATOM | 863 | CG2 | ILE | A | 93 | -8.022 | 9.486 | 24.735 |
| ATOM | 864 | CD1 | ILE | A | 93 | -5.754 | 7.740 | 25.693 |
| ATOM | 865 | N | GLY | A | 94 | -4.594 | 12.993 | 25.330 |
| ATOM | 866 | H | GLY | A | 94 | -4.617 | 13.079 | 24.334 |
| ATOM | 867 | CA | GLY | A | 94 | -3.613 | 13.742 | 26.063 |
| ATOM | 868 | C | GLY | A | 94 | -2.448 | 12.895 | 26.512 |
| ATOM | 869 | O | GLY | A | 94 | -1.764 | 13.158 | 27.519 |
| ATOM | 870 | N | CYS | A | 95 | -2.117 | 11.849 | 25.797 |
| ATOM | 871 | H | CYS | A | 95 | -2.619 | 11.644 | 24.957 |
| ATOM | 872 | CA | CYS | A | 95 | -1.036 | 10.994 | 26.214 |
| ATOM | 873 | C | CYS | A | 95 | 0.362 | 11.566 | 25.925 |
| ATOM | 874 | O | CYS | A | 95 | 0.588 | 12.254 | 24.907 |
| ATOM | 875 | CB | CYS | A | 95 | -1.260 | 9.655 | 25.550 |
| ATOM | 876 | SG | CYS | A | 95 | -0.254 | 8.307 | 26.125 |
| ATOM | 877 | N | THR | A | 96 | 1.346 | 11.297 | 26.803 |
| ATOM | 878 | H | THR | A | 96 | 1.135 | 10.738 | 27.618 |
| ATOM | 879 | CA | THR | A | 96 | 2.728 | 11.779 | 26.664 |
| ATOM | 880 | C | THR | A | 96 | 3.729 | 10.784 | 27.264 |
| ATOM | 881 | O | THR | A | 96 | 3.498 | 10.249 | 28.345 |
| ATOM | 882 | CB | THR | A | 96 | 2.925 | 13.154 | 27.346 |
| ATOM | 883 | OG1 | THR | A | 96 | 2.594 | 13.109 | 28.721 |
| ATOM | 884 | HG1 | THR | A | 96 | 2.784 | 13.966 | 29.109 |
| ATOM | 885 | CG2 | THR | A | 96 | 2.139 | 14.300 | 26.698 |
| ATOM | 886 | N | LEU | A | 97 | 4.882 | 10.603 | 26.599 |
| ATOM | 887 | H | LEU | A | 97 | 5.016 | 11.071 | 25.714 |
| ATOM | 888 | CA | LEU | A | 97 | 6.040 | 9.910 | 27.166 |
| ATOM | 889 | C | LEU | A | 97 | 6.751 | 10.824 | 28.175 |
| ATOM | 890 | O | LEU | A | 97 | 6.705 | 12.046 | 28.044 |
| ATOM | 891 | CB | LEU | A | 97 | 7.013 | 9.497 | 26.049 |
| ATOM | 892 | CG | LEU | A | 97 | 6.452 | 8.449 | 25.065 |
| ATOM | 893 | CD1 | LEU | A | 97 | 7.360 | 8.355 | 23.828 |
| ATOM | 894 | CD2 | LEU | A | 97 | 6.345 | 7.065 | 25.724 |
| ATOM | 895 | N | ASN | A | 98 | 7.412 | 10.221 | 29.175 |

FIG. 1 IP

```
ATOM    896   H   ASN A  98       7.413   9.212  29.205
ATOM    897   CA  ASN A  98       8.065  10.897  30.292
ATOM    898   C   ASN A  98       9.220  10.029  30.800
ATOM    899   O   ASN A  98       8.995   9.079  31.550
ATOM    900   CB  ASN A  98       7.057  11.177  31.423
ATOM    901   CG  ASN A  98       6.084  12.305  31.083
ATOM    902   OD1 ASN A  98       4.983  12.062  30.594
ATOM    903   ND2 ASN A  98       6.493  13.549  31.342
ATOM    904  2HD2 ASN A  98       5.888  14.331  31.136
ATOM    905  1HD2 ASN A  98       7.406  13.707  31.742
ATOM    906   N   LEU A  99      10.451  10.369  30.389
ATOM    907   H   LEU A  99      10.547  11.177  29.792
ATOM    908   CA  LEU A  99      11.679   9.620  30.666
ATOM    909   C   LEU A  99      12.711  10.437  31.454
ATOM    910   O   LEU A  99      12.487  11.652  31.651
ATOM    911   CB  LEU A  99      12.233   8.989  29.369
ATOM    912   CG  LEU A  99      12.833   9.873  28.248
ATOM    913   CD1 LEU A  99      11.876  10.947  27.705
ATOM    914   CD2 LEU A  99      14.183  10.505  28.623
ATOM    915   OXT LEU A  99      13.716   9.819  31.869
TER
ATOM    916   N   PRO B   1      12.600  14.237  30.106
ATOM    917   CA  PRO B   1      11.842  15.268  29.363
ATOM    918   C   PRO B   1      10.430  14.773  29.138
ATOM    919   O   PRO B   1      10.054  13.695  29.618
ATOM    920   CB  PRO B   1      12.622  15.412  28.035
ATOM    921   CG  PRO B   1      13.817  14.470  28.131
ATOM    922   CD  PRO B   1      13.966  14.227  29.603
ATOM    923  1H   PRO B   1      12.175  13.343  29.964
ATOM    924  2H   PRO B   1      12.594  14.457  31.081
ATOM    925   N   GLN B   2       9.513  15.542  28.523
ATOM    926   H   GLN B   2       9.751  16.474  28.251
ATOM    927   CA  GLN B   2       8.186  15.058  28.242
ATOM    928   C   GLN B   2       8.066  15.151  26.749
ATOM    929   O   GLN B   2       8.523  16.140  26.133
ATOM    930   CB  GLN B   2       7.155  15.976  28.856
ATOM    931   CG  GLN B   2       5.739  15.732  28.373
ATOM    932   CD  GLN B   2       4.744  16.365  29.284
ATOM    933   OE1 GLN B   2       4.628  15.962  30.431
ATOM    934   NE2 GLN B   2       4.024  17.367  28.784
ATOM    935  1HE2 GLN B   2       3.341  17.830  29.349
ATOM    936  2HE2 GLN B   2       4.160  17.665  27.839
ATOM    937   N   ILE B   3       7.499  14.176  26.036
ATOM    938   H   ILE B   3       7.102  13.386  26.504
ATOM    939   CA  ILE B   3       7.435  14.216  24.601
ATOM    940   C   ILE B   3       5.956  14.097  24.184
ATOM    941   O   ILE B   3       5.150  13.290  24.710
ATOM    942   CB  ILE B   3       8.299  13.058  24.029
ATOM    943   CG1 ILE B   3       9.743  13.232  24.534
ATOM    944   CG2 ILE B   3       8.269  12.985  22.496
ATOM    945   CD1 ILE B   3      10.621  12.068  24.143
ATOM    946   N   THR B   4       5.462  15.108  23.453
ATOM    947   H   THR B   4       6.046  15.887  23.226
ATOM    948   CA  THR B   4       4.107  15.115  22.976
ATOM    949   C   THR B   4       4.039  14.193  21.765
ATOM    950   O   THR B   4       5.066  13.755  21.203
```

FIG. 1Q

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 951 | CB | THR | B | 4 | 3.616 | 16.548 | 22.647 |
| ATOM | 952 | OG1 | THR | B | 4 | 4.450 | 17.157 | 21.645 |
| ATOM | 953 | HG1 | THR | B | 4 | 4.123 | 18.080 | 21.442 |
| ATOM | 954 | CG2 | THR | B | 4 | 3.644 | 17.454 | 23.876 |
| ATOM | 955 | N | LEU | B | 5 | 2.872 | 13.781 | 21.324 |
| ATOM | 956 | H | LEU | B | 5 | 2.033 | 14.151 | 21.723 |
| ATOM | 957 | CA | LEU | B | 5 | 2.837 | 12.795 | 20.265 |
| ATOM | 958 | C | LEU | B | 5 | 2.183 | 13.415 | 19.047 |
| ATOM | 959 | O | LEU | B | 5 | 1.677 | 12.720 | 18.142 |
| ATOM | 960 | CB | LEU | B | 5 | 2.093 | 11.577 | 20.762 |
| ATOM | 961 | CG | LEU | B | 5 | 2.819 | 10.856 | 21.892 |
| ATOM | 962 | CD1 | LEU | B | 5 | 1.889 | 9.885 | 22.602 |
| ATOM | 963 | CD2 | LEU | B | 5 | 4.108 | 10.159 | 21.416 |
| ATOM | 964 | N | TRP | B | 6 | 2.209 | 14.742 | 18.880 |
| ATOM | 965 | H | TRP | B | 6 | 2.601 | 15.323 | 19.593 |
| ATOM | 966 | CA | TRP | B | 6 | 1.683 | 15.364 | 17.690 |
| ATOM | 967 | C | TRP | B | 6 | 2.581 | 14.978 | 16.509 |
| ATOM | 968 | O | TRP | B | 6 | 2.159 | 14.851 | 15.349 |
| ATOM | 969 | CB | TRP | B | 6 | 1.587 | 16.879 | 17.833 |
| ATOM | 970 | CG | TRP | B | 6 | 0.652 | 17.339 | 18.921 |
| ATOM | 971 | CD1 | TRP | B | 6 | 0.955 | 17.584 | 20.232 |
| ATOM | 972 | CD2 | TRP | B | 6 | -0.750 | 17.612 | 18.783 |
| ATOM | 973 | NE1 | TRP | B | 6 | -0.167 | 17.989 | 20.913 |
| ATOM | 974 | HE1 | TRP | B | 6 | -0.217 | 18.230 | 21.882 |
| ATOM | 975 | CE2 | TRP | B | 6 | -1.224 | 18.013 | 20.048 |
| ATOM | 976 | CE3 | TRP | B | 6 | -1.637 | 17.550 | 17.709 |
| ATOM | 977 | CZ2 | TRP | B | 6 | -2.544 | 18.352 | 20.266 |
| ATOM | 978 | CZ3 | TRP | B | 6 | -2.947 | 17.885 | 17.921 |
| ATOM | 979 | CH2 | TRP | B | 6 | -3.394 | 18.281 | 19.185 |
| ATOM | 980 | N | GLN | B | 7 | 3.896 | 14.809 | 16.738 |
| ATOM | 981 | H | GLN | B | 7 | 4.267 | 14.985 | 17.650 |
| ATOM | 982 | CA | GLN | B | 7 | 4.794 | 14.376 | 15.689 |
| ATOM | 983 | C | GLN | B | 7 | 5.361 | 13.043 | 16.096 |
| ATOM | 984 | O | GLN | B | 7 | 5.221 | 12.586 | 17.243 |
| ATOM | 985 | CB | GLN | B | 7 | 5.880 | 15.430 | 15.505 |
| ATOM | 986 | CG | GLN | B | 7 | 5.353 | 16.704 | 14.804 |
| ATOM | 987 | CD | GLN | B | 7 | 6.197 | 17.912 | 15.137 |
| ATOM | 988 | OE1 | GLN | B | 7 | 7.400 | 17.802 | 15.404 |
| ATOM | 989 | NE2 | GLN | B | 7 | 5.553 | 19.083 | 15.121 |
| ATOM | 990 | 1HE2 | GLN | B | 7 | 6.040 | 19.931 | 15.330 |
| ATOM | 991 | 2HE2 | GLN | B | 7 | 4.579 | 19.121 | 14.900 |
| ATOM | 992 | N | ARG | B | 8 | 5.979 | 12.274 | 15.189 |
| ATOM | 993 | H | ARG | B | 8 | 6.073 | 12.597 | 14.247 |
| ATOM | 994 | CA | ARG | B | 8 | 6.505 | 10.985 | 15.573 |
| ATOM | 995 | C | ARG | B | 8 | 7.577 | 11.198 | 16.610 |
| ATOM | 996 | O | ARG | B | 8 | 8.395 | 12.130 | 16.515 |
| ATOM | 997 | CB | ARG | B | 8 | 7.092 | 10.238 | 14.384 |
| ATOM | 998 | CG | ARG | B | 8 | 6.132 | 10.018 | 13.237 |
| ATOM | 999 | CD | ARG | B | 8 | 6.802 | 9.402 | 12.046 |
| ATOM | 1000 | NE | ARG | B | 8 | 5.846 | 9.005 | 11.023 |
| ATOM | 1001 | HE | ARG | B | 8 | 4.872 | 9.080 | 11.237 |
| ATOM | 1002 | CZ | ARG | B | 8 | 6.217 | 8.552 | 9.828 |
| ATOM | 1003 | NH1 | ARG | B | 8 | 7.496 | 8.442 | 9.486 |
| ATOM | 1004 | 2HH1 | ARG | B | 8 | 8.211 | 8.703 | 10.134 |
| ATOM | 1005 | 1HH1 | ARG | B | 8 | 7.744 | 8.098 | 8.580 |
| ATOM | 1006 | NH2 | ARG | B | 8 | 5.279 | 8.202 | 8.952 |

FIG. 1IR

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1007 | 1HH2 | ARG | B | 8 | 5.540 | 7.860 | 8.050 |
| ATOM | 1008 | 2HH2 | ARG | B | 8 | 4.312 | 8.281 | 9.196 |
| ATOM | 1009 | N | PRO | B | 9 | 7.663 | 10.381 | 17.682 |
| ATOM | 1010 | CA | PRO | B | 9 | 8.666 | 10.587 | 18.746 |
| ATOM | 1011 | C | PRO | B | 9 | 10.065 | 10.196 | 18.315 |
| ATOM | 1012 | O | PRO | B | 9 | 10.678 | 9.215 | 18.778 |
| ATOM | 1013 | CB | PRO | B | 9 | 8.148 | 9.682 | 19.878 |
| ATOM | 1014 | CG | PRO | B | 9 | 7.315 | 8.607 | 19.206 |
| ATOM | 1015 | CD | PRO | B | 9 | 6.708 | 9.323 | 18.004 |
| ATOM | 1016 | N | LEU | B | 10 | 10.685 | 10.969 | 17.400 |
| ATOM | 1017 | H | LEU | B | 10 | 10.201 | 11.746 | 16.998 |
| ATOM | 1018 | CA | LEU | B | 10 | 12.040 | 10.706 | 16.978 |
| ATOM | 1019 | C | LEU | B | 10 | 12.976 | 11.498 | 17.850 |
| ATOM | 1020 | O | LEU | B | 10 | 12.880 | 12.733 | 18.018 |
| ATOM | 1021 | CB | LEU | B | 10 | 12.250 | 11.170 | 15.554 |
| ATOM | 1022 | CG | LEU | B | 10 | 11.427 | 10.386 | 14.551 |
| ATOM | 1023 | CD1 | LEU | B | 10 | 11.385 | 11.175 | 13.276 |
| ATOM | 1024 | CD2 | LEU | B | 10 | 11.956 | 8.947 | 14.355 |
| ATOM | 1025 | N | VAL | B | 11 | 14.030 | 10.843 | 18.384 |
| ATOM | 1026 | H | VAL | B | 11 | 14.148 | 9.866 | 18.206 |
| ATOM | 1027 | CA | VAL | B | 11 | 15.018 | 11.517 | 19.223 |
| ATOM | 1028 | C | VAL | B | 11 | 16.400 | 11.111 | 18.740 |
| ATOM | 1029 | O | VAL | B | 11 | 16.581 | 10.201 | 17.911 |
| ATOM | 1030 | CB | VAL | B | 11 | 14.857 | 11.100 | 20.699 |
| ATOM | 1031 | CG1 | VAL | B | 11 | 13.514 | 11.586 | 21.293 |
| ATOM | 1032 | CG2 | VAL | B | 11 | 15.038 | 9.573 | 20.903 |
| ATOM | 1033 | N | THR | B | 12 | 17.485 | 11.739 | 19.232 |
| ATOM | 1034 | H | THR | B | 12 | 17.370 | 12.507 | 19.862 |
| ATOM | 1035 | CA | THR | B | 12 | 18.843 | 11.325 | 18.868 |
| ATOM | 1036 | C | THR | B | 12 | 19.377 | 10.284 | 19.837 |
| ATOM | 1037 | O | THR | B | 12 | 19.237 | 10.352 | 21.082 |
| ATOM | 1038 | CB | THR | B | 12 | 19.830 | 12.520 | 18.820 |
| ATOM | 1039 | OG1 | THR | B | 12 | 19.389 | 13.483 | 17.876 |
| ATOM | 1040 | HG1 | THR | B | 12 | 20.028 | 14.252 | 17.848 |
| ATOM | 1041 | CG2 | THR | B | 12 | 21.234 | 12.075 | 18.399 |
| ATOM | 1042 | N | ILE | B | 13 | 20.044 | 9.234 | 19.338 |
| ATOM | 1043 | H | ILE | B | 13 | 20.135 | 9.130 | 18.348 |
| ATOM | 1044 | CA | ILE | B | 13 | 20.641 | 8.239 | 20.176 |
| ATOM | 1045 | C | ILE | B | 13 | 22.119 | 8.226 | 19.855 |
| ATOM | 1046 | O | ILE | B | 13 | 22.579 | 8.817 | 18.865 |
| ATOM | 1047 | CB | ILE | B | 13 | 19.993 | 6.870 | 19.879 |
| ATOM | 1048 | CG1 | ILE | B | 13 | 20.192 | 6.464 | 18.415 |
| ATOM | 1049 | CG2 | ILE | B | 13 | 18.482 | 6.893 | 20.206 |
| ATOM | 1050 | CD1 | ILE | B | 13 | 19.829 | 5.035 | 18.106 |
| ATOM | 1051 | N | LYS | B | 14 | 22.973 | 7.618 | 20.661 |
| ATOM | 1052 | H | LYS | B | 14 | 22.652 | 7.243 | 21.531 |
| ATOM | 1053 | CA | LYS | B | 14 | 24.364 | 7.480 | 20.317 |
| ATOM | 1054 | C | LYS | B | 14 | 24.680 | 6.029 | 20.477 |
| ATOM | 1055 | O | LYS | B | 14 | 24.353 | 5.353 | 21.484 |
| ATOM | 1056 | CB | LYS | B | 14 | 25.266 | 8.263 | 21.242 |
| ATOM | 1057 | CG | LYS | B | 14 | 24.947 | 9.729 | 21.236 |
| ATOM | 1058 | CD | LYS | B | 14 | 25.664 | 10.498 | 22.339 |
| ATOM | 1059 | CE | LYS | B | 14 | 26.758 | 11.441 | 21.807 |
| ATOM | 1060 | NZ | LYS | B | 14 | 28.026 | 10.781 | 21.440 |
| ATOM | 1061 | 1HZ | LYS | B | 14 | 28.674 | 11.466 | 21.107 |
| ATOM | 1062 | 3HZ | LYS | B | 14 | 27.855 | 10.107 | 20.722 |

FIG. 1 IS

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1063 | 2HZ | LYS | B | 14 | 28.408 | 10.323 | 22.243 |
| ATOM | 1064 | N | ILE | B | 15 | 25.214 | 5.390 | 19.425 |
| ATOM | 1065 | H | ILE | B | 15 | 25.434 | 5.901 | 18.594 |
| ATOM | 1066 | CA | ILE | B | 15 | 25.489 | 3.989 | 19.434 |
| ATOM | 1067 | C | ILE | B | 15 | 26.832 | 3.981 | 18.750 |
| ATOM | 1068 | O | ILE | B | 15 | 27.104 | 4.869 | 17.933 |
| ATOM | 1069 | CB | ILE | B | 15 | 24.435 | 3.220 | 18.606 |
| ATOM | 1070 | CG1 | ILE | B | 15 | 24.893 | 1.824 | 18.347 |
| ATOM | 1071 | CG2 | ILE | B | 15 | 24.048 | 3.977 | 17.309 |
| ATOM | 1072 | CD1 | ILE | B | 15 | 23.830 | 0.996 | 17.645 |
| ATOM | 1073 | N | GLY | B | 16 | 27.812 | 3.212 | 19.202 |
| ATOM | 1074 | H | GLY | B | 16 | 27.623 | 2.535 | 19.913 |
| ATOM | 1075 | CA | GLY | B | 16 | 29.175 | 3.336 | 18.677 |
| ATOM | 1076 | C | GLY | B | 16 | 29.771 | 4.754 | 18.619 |
| ATOM | 1077 | O | GLY | B | 16 | 30.737 | 4.970 | 17.902 |
| ATOM | 1078 | N | GLY | B | 17 | 29.273 | 5.791 | 19.335 |
| ATOM | 1079 | H | GLY | B | 17 | 28.453 | 5.660 | 19.892 |
| ATOM | 1080 | CA | GLY | B | 17 | 29.924 | 7.105 | 19.302 |
| ATOM | 1081 | C | GLY | B | 17 | 29.468 | 8.043 | 18.176 |
| ATOM | 1082 | O | GLY | B | 17 | 29.984 | 9.155 | 17.933 |
| ATOM | 1083 | N | GLN | B | 18 | 28.433 | 7.621 | 17.411 |
| ATOM | 1084 | H | GLN | B | 18 | 28.046 | 6.711 | 17.560 |
| ATOM | 1085 | CA | GLN | B | 18 | 27.834 | 8.449 | 16.348 |
| ATOM | 1086 | C | GLN | B | 18 | 26.407 | 8.755 | 16.736 |
| ATOM | 1087 | O | GLN | B | 18 | 25.678 | 7.953 | 17.353 |
| ATOM | 1088 | CB | GLN | B | 18 | 27.810 | 7.645 | 15.045 |
| ATOM | 1089 | CG | GLN | B | 18 | 27.247 | 6.204 | 15.146 |
| ATOM | 1090 | CD | GLN | B | 18 | 27.572 | 5.333 | 13.924 |
| ATOM | 1091 | OE1 | GLN | B | 18 | 26.771 | 4.501 | 13.464 |
| ATOM | 1092 | NE2 | GLN | B | 18 | 28.766 | 5.531 | 13.393 |
| ATOM | 1093 | 1HE2 | GLN | B | 18 | 29.057 | 5.005 | 12.594 |
| ATOM | 1094 | 2HE2 | GLN | B | 18 | 29.388 | 6.209 | 13.786 |
| ATOM | 1095 | N | LEU | B | 19 | 25.873 | 9.933 | 16.337 |
| ATOM | 1096 | H | LEU | B | 19 | 26.446 | 10.602 | 15.863 |
| ATOM | 1097 | CA | LEU | B | 19 | 24.467 | 10.267 | 16.578 |
| ATOM | 1098 | C | LEU | B | 19 | 23.633 | 9.622 | 15.490 |
| ATOM | 1099 | O | LEU | B | 19 | 23.912 | 9.707 | 14.284 |
| ATOM | 1100 | CB | LEU | B | 19 | 24.207 | 11.777 | 16.457 |
| ATOM | 1101 | CG | LEU | B | 19 | 24.857 | 12.756 | 17.454 |
| ATOM | 1102 | CD1 | LEU | B | 19 | 24.739 | 12.335 | 18.880 |
| ATOM | 1103 | CD2 | LEU | B | 19 | 26.299 | 13.072 | 17.130 |
| ATOM | 1104 | N | LYS | B | 20 | 22.450 | 9.085 | 15.850 |
| ATOM | 1105 | H | LYS | B | 20 | 22.242 | 8.948 | 16.819 |
| ATOM | 1106 | CA | LYS | B | 20 | 21.472 | 8.702 | 14.867 |
| ATOM | 1107 | C | LYS | B | 20 | 20.121 | 9.105 | 15.417 |
| ATOM | 1108 | O | LYS | B | 20 | 19.957 | 9.572 | 16.569 |
| ATOM | 1109 | CB | LYS | B | 20 | 21.496 | 7.200 | 14.560 |
| ATOM | 1110 | CG | LYS | B | 20 | 22.904 | 6.653 | 14.507 |
| ATOM | 1111 | CD | LYS | B | 20 | 23.052 | 5.366 | 13.677 |
| ATOM | 1112 | CE | LYS | B | 20 | 23.069 | 5.603 | 12.145 |
| ATOM | 1113 | NZ | LYS | B | 20 | 23.893 | 6.758 | 11.699 |
| ATOM | 1114 | 1HZ | LYS | B | 20 | 23.847 | 6.836 | 10.703 |
| ATOM | 1115 | 3HZ | LYS | B | 20 | 24.843 | 6.617 | 11.978 |
| ATOM | 1116 | 2HZ | LYS | B | 20 | 23.544 | 7.597 | 12.116 |
| ATOM | 1117 | N | GLU | B | 21 | 19.068 | 9.022 | 14.591 |
| ATOM | 1118 | H | GLU | B | 21 | 19.200 | 8.712 | 13.650 |

FIG. 11T

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1119 | CA | GLU | B | 21 | 17.735 | 9.366 | 15.008 |
| ATOM | 1120 | C | GLU | B | 21 | 16.937 | 8.095 | 15.119 |
| ATOM | 1121 | O | GLU | B | 21 | 17.117 | 7.103 | 14.376 |
| ATOM | 1122 | CB | GLU | B | 21 | 17.143 | 10.314 | 13.983 |
| ATOM | 1123 | CG | GLU | B | 21 | 15.714 | 10.706 | 14.162 |
| ATOM | 1124 | CD | GLU | B | 21 | 15.304 | 11.607 | 13.036 |
| ATOM | 1125 | OE1 | GLU | B | 21 | 14.971 | 11.051 | 11.957 |
| ATOM | 1126 | OE2 | GLU | B | 21 | 15.338 | 12.854 | 13.174 |
| ATOM | 1127 | N | ALA | B | 22 | 16.025 | 7.999 | 16.072 |
| ATOM | 1128 | H | ALA | B | 22 | 15.825 | 8.792 | 16.648 |
| ATOM | 1129 | CA | ALA | B | 22 | 15.300 | 6.783 | 16.315 |
| ATOM | 1130 | C | ALA | B | 22 | 13.981 | 7.132 | 16.952 |
| ATOM | 1131 | O | ALA | B | 22 | 13.756 | 8.153 | 17.632 |
| ATOM | 1132 | CB | ALA | B | 22 | 16.095 | 5.865 | 17.235 |
| ATOM | 1133 | N | LEU | B | 23 | 12.994 | 6.230 | 16.743 |
| ATOM | 1134 | H | LEU | B | 23 | 13.195 | 5.379 | 16.257 |
| ATOM | 1135 | CA | LEU | B | 23 | 11.639 | 6.408 | 17.180 |
| ATOM | 1136 | C | LEU | B | 23 | 11.476 | 5.740 | 18.534 |
| ATOM | 1137 | O | LEU | B | 23 | 11.814 | 4.564 | 18.746 |
| ATOM | 1138 | CB | LEU | B | 23 | 10.775 | 5.665 | 16.192 |
| ATOM | 1139 | CG | LEU | B | 23 | 9.267 | 5.810 | 16.237 |
| ATOM | 1140 | CD1 | LEU | B | 23 | 8.807 | 7.142 | 15.664 |
| ATOM | 1141 | CD2 | LEU | B | 23 | 8.648 | 4.625 | 15.482 |
| ATOM | 1142 | N | LEU | B | 24 | 10.948 | 6.455 | 19.553 |
| ATOM | 1143 | H | LEU | B | 24 | 10.775 | 7.433 | 19.435 |
| ATOM | 1144 | CA | LEU | B | 24 | 10.613 | 5.838 | 20.849 |
| ATOM | 1145 | C | LEU | B | 24 | 9.271 | 5.160 | 20.687 |
| ATOM | 1146 | O | LEU | B | 24 | 8.208 | 5.764 | 20.418 |
| ATOM | 1147 | CB | LEU | B | 24 | 10.564 | 6.878 | 21.971 |
| ATOM | 1148 | CG | LEU | B | 24 | 11.828 | 7.750 | 22.075 |
| ATOM | 1149 | CD1 | LEU | B | 24 | 11.580 | 8.859 | 23.077 |
| ATOM | 1150 | CD2 | LEU | B | 24 | 13.099 | 6.955 | 22.388 |
| ATOM | 1151 | N | ASP | B | 25 | 9.246 | 3.822 | 20.809 |
| ATOM | 1152 | H | ASP | B | 25 | 10.025 | 3.347 | 21.218 |
| ATOM | 1153 | CA | ASP | B | 25 | 8.122 | 3.030 | 20.366 |
| ATOM | 1154 | C | ASP | B | 25 | 7.637 | 2.136 | 21.484 |
| ATOM | 1155 | O | ASP | B | 25 | 8.189 | 1.048 | 21.759 |
| ATOM | 1156 | CB | ASP | B | 25 | 8.613 | 2.196 | 19.189 |
| ATOM | 1157 | CG | ASP | B | 25 | 7.528 | 1.421 | 18.511 |
| ATOM | 1158 | OD1 | ASP | B | 25 | 6.422 | 1.339 | 19.058 |
| ATOM | 1159 | OD2 | ASP | B | 25 | 7.800 | 0.897 | 17.426 |
| ATOM | 1160 | N | THR | B | 26 | 6.547 | 2.465 | 22.157 |
| ATOM | 1161 | H | THR | B | 26 | 6.067 | 3.314 | 21.938 |
| ATOM | 1162 | CA | THR | B | 26 | 6.025 | 1.621 | 23.212 |
| ATOM | 1163 | C | THR | B | 26 | 5.347 | 0.369 | 22.694 |
| ATOM | 1164 | O | THR | B | 26 | 4.976 | -0.550 | 23.451 |
| ATOM | 1165 | CB | THR | B | 26 | 5.027 | 2.389 | 24.046 |
| ATOM | 1166 | OG1 | THR | B | 26 | 3.927 | 2.853 | 23.239 |
| ATOM | 1167 | HG1 | THR | B | 26 | 3.277 | 3.359 | 23.806 |
| ATOM | 1168 | CG2 | THR | B | 26 | 5.703 | 3.603 | 24.650 |
| ATOM | 1169 | N | GLY | B | 27 | 5.090 | 0.245 | 21.382 |
| ATOM | 1170 | H | GLY | B | 27 | 5.341 | 0.983 | 20.756 |
| ATOM | 1171 | CA | GLY | B | 27 | 4.457 | -0.938 | 20.867 |
| ATOM | 1172 | C | GLY | B | 27 | 5.475 | -1.992 | 20.458 |
| ATOM | 1173 | O | GLY | B | 27 | 5.121 | -3.108 | 20.055 |
| ATOM | 1174 | N | ALA | B | 28 | 6.792 | -1.717 | 20.495 |

FIG. 1 IU

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1175 | H | ALA | B | 28 | 7.104 | -0.832 | 20.841 |
| ATOM | 1176 | CA | ALA | B | 28 | 7.800 | -2.690 | 20.037 |
| ATOM | 1177 | C | ALA | B | 28 | 8.371 | -3.444 | 21.259 |
| ATOM | 1178 | O | ALA | B | 28 | 8.840 | -2.807 | 22.213 |
| ATOM | 1179 | CB | ALA | B | 28 | 8.924 | -1.936 | 19.358 |
| ATOM | 1180 | N | ASP | B | 29 | 8.459 | -4.787 | 21.289 |
| ATOM | 1181 | H | ASP | B | 29 | 8.082 | -5.325 | 20.535 |
| ATOM | 1182 | CA | ASP | B | 29 | 9.121 | -5.441 | 22.452 |
| ATOM | 1183 | C | ASP | B | 29 | 10.608 | -5.219 | 22.404 |
| ATOM | 1184 | O | ASP | B | 29 | 11.345 | -5.264 | 23.412 |
| ATOM | 1185 | CB | ASP | B | 29 | 8.965 | -6.975 | 22.447 |
| ATOM | 1186 | CG | ASP | B | 29 | 7.551 | -7.477 | 22.774 |
| ATOM | 1187 | OD1 | ASP | B | 29 | 6.683 | -6.693 | 23.169 |
| ATOM | 1188 | OD2 | ASP | B | 29 | 7.350 | -8.686 | 22.616 |
| ATOM | 1189 | N | ASP | B | 30 | 11.164 | -5.157 | 21.171 |
| ATOM | 1190 | H | ASP | B | 30 | 10.577 | -5.063 | 20.367 |
| ATOM | 1191 | CA | ASP | B | 30 | 12.609 | -5.217 | 20.880 |
| ATOM | 1192 | C | ASP | B | 30 | 13.048 | -3.886 | 20.335 |
| ATOM | 1193 | O | ASP | B | 30 | 12.269 | -3.055 | 19.817 |
| ATOM | 1194 | CB | ASP | B | 30 | 12.833 | -6.226 | 19.735 |
| ATOM | 1195 | CG | ASP | B | 30 | 12.477 | -7.675 | 20.099 |
| ATOM | 1196 | OD1 | ASP | B | 30 | 13.197 | -8.272 | 20.908 |
| ATOM | 1197 | OD2 | ASP | B | 30 | 11.494 | -8.237 | 19.569 |
| ATOM | 1198 | N | THR | B | 31 | 14.387 | -3.692 | 20.227 |
| ATOM | 1199 | H | THR | B | 31 | 15.018 | -4.380 | 20.586 |
| ATOM | 1200 | CA | THR | B | 31 | 14.981 | -2.530 | 19.614 |
| ATOM | 1201 | C | THR | B | 31 | 15.578 | -2.979 | 18.260 |
| ATOM | 1202 | O | THR | B | 31 | 16.246 | -4.020 | 18.123 |
| ATOM | 1203 | CB | THR | B | 31 | 16.036 | -2.004 | 20.557 |
| ATOM | 1204 | OG1 | THR | B | 31 | 15.378 | -1.376 | 21.645 |
| ATOM | 1205 | HG1 | THR | B | 31 | 16.052 | -1.016 | 22.290 |
| ATOM | 1206 | CG2 | THR | B | 31 | 16.944 | -0.960 | 19.904 |
| ATOM | 1207 | N | VAL | B | 32 | 15.237 | -2.283 | 17.150 |
| ATOM | 1208 | H | VAL | B | 32 | 14.703 | -1.442 | 17.237 |
| ATOM | 1209 | CA | VAL | B | 32 | 15.626 | -2.722 | 15.806 |
| ATOM | 1210 | C | VAL | B | 32 | 16.303 | -1.566 | 15.132 |
| ATOM | 1211 | O | VAL | B | 32 | 15.779 | -0.428 | 14.995 |
| ATOM | 1212 | CB | VAL | B | 32 | 14.407 | -3.126 | 14.964 |
| ATOM | 1213 | CG1 | VAL | B | 32 | 14.820 | -3.703 | 13.596 |
| ATOM | 1214 | CG2 | VAL | B | 32 | 13.556 | -4.102 | 15.703 |
| ATOM | 1215 | N | LEU | B | 33 | 17.563 | -1.756 | 14.720 |
| ATOM | 1216 | H | LEU | B | 33 | 17.984 | -2.658 | 14.814 |
| ATOM | 1217 | CA | LEU | B | 33 | 18.347 | -0.697 | 14.138 |
| ATOM | 1218 | C | LEU | B | 33 | 18.610 | -1.009 | 12.685 |
| ATOM | 1219 | O | LEU | B | 33 | 18.685 | -2.162 | 12.205 |
| ATOM | 1220 | CB | LEU | B | 33 | 19.679 | -0.628 | 14.856 |
| ATOM | 1221 | CG | LEU | B | 33 | 19.698 | 0.363 | 16.031 |
| ATOM | 1222 | CD1 | LEU | B | 33 | 18.425 | 0.321 | 16.891 |
| ATOM | 1223 | CD2 | LEU | B | 33 | 20.929 | 0.179 | 16.889 |
| ATOM | 1224 | N | GLU | B | 34 | 18.786 | 0.078 | 11.899 |
| ATOM | 1225 | H | GLU | B | 34 | 18.619 | 0.991 | 12.271 |
| ATOM | 1226 | CA | GLU | B | 34 | 19.218 | 0.041 | 10.488 |
| ATOM | 1227 | C | GLU | B | 34 | 20.478 | -0.774 | 10.399 |
| ATOM | 1228 | O | GLU | B | 34 | 21.374 | -0.835 | 11.272 |
| ATOM | 1229 | CB | GLU | B | 34 | 19.536 | 1.460 | 9.996 |
| ATOM | 1230 | CG | GLU | B | 34 | 20.722 | 2.088 | 10.761 |

FIG. 1IV

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1231 | CD | GLU | B | 34 | 21.085 | 3.512 | 10.314 |
| ATOM | 1232 | OE1 | GLU | B | 34 | 20.285 | 4.466 | 10.500 |
| ATOM | 1233 | OE2 | GLU | B | 34 | 22.211 | 3.703 | 9.775 |
| ATOM | 1234 | N | GLU | B | 35 | 20.673 | -1.367 | 9.205 |
| ATOM | 1235 | H | GLU | B | 35 | 20.011 | -1.227 | 8.468 |
| ATOM | 1236 | CA | GLU | B | 35 | 21.802 | -2.205 | 8.930 |
| ATOM | 1237 | C | GLU | B | 35 | 23.096 | -1.520 | 9.321 |
| ATOM | 1238 | O | GLU | B | 35 | 23.391 | -0.379 | 8.916 |
| ATOM | 1239 | CB | GLU | B | 35 | 21.741 | -2.479 | 7.439 |
| ATOM | 1240 | CG | GLU | B | 35 | 22.795 | -3.380 | 6.883 |
| ATOM | 1241 | CD | GLU | B | 35 | 22.987 | -4.587 | 7.744 |
| ATOM | 1242 | OE1 | GLU | B | 35 | 21.980 | -5.258 | 8.118 |
| ATOM | 1243 | OE2 | GLU | B | 35 | 24.149 | -4.860 | 8.048 |
| ATOM | 1244 | N | MET | B | 36 | 23.926 | -2.106 | 10.157 |
| ATOM | 1245 | H | MET | B | 36 | 23.654 | -2.953 | 10.613 |
| ATOM | 1246 | CA | MET | B | 36 | 25.232 | -1.559 | 10.441 |
| ATOM | 1247 | C | MET | B | 36 | 26.146 | -2.687 | 10.815 |
| ATOM | 1248 | O | MET | B | 36 | 25.731 | -3.783 | 11.257 |
| ATOM | 1249 | CB | MET | B | 36 | 25.251 | -0.424 | 11.497 |
| ATOM | 1250 | CG | MET | B | 36 | 24.626 | -0.724 | 12.881 |
| ATOM | 1251 | SD | MET | B | 36 | 24.722 | 0.719 | 13.988 |
| ATOM | 1252 | CE | MET | B | 36 | 23.132 | 1.586 | 13.692 |
| ATOM | 1253 | N | SER | B | 37 | 27.441 | -2.551 | 10.593 |
| ATOM | 1254 | H | SER | B | 37 | 27.783 | -1.726 | 10.144 |
| ATOM | 1255 | CA | SER | B | 37 | 28.321 | -3.608 | 11.011 |
| ATOM | 1256 | C | SER | B | 37 | 28.721 | -3.352 | 12.442 |
| ATOM | 1257 | O | SER | B | 37 | 29.402 | -2.369 | 12.788 |
| ATOM | 1258 | CB | SER | B | 37 | 29.567 | -3.622 | 10.109 |
| ATOM | 1259 | OG | SER | B | 37 | 29.231 | -3.908 | 8.750 |
| ATOM | 1260 | HG | SER | B | 37 | 30.057 | -3.911 | 8.187 |
| ATOM | 1261 | N | LEU | B | 38 | 28.469 | -4.295 | 13.366 |
| ATOM | 1262 | H | LEU | B | 38 | 27.948 | -5.123 | 13.117 |
| ATOM | 1263 | CA | LEU | B | 38 | 29.073 | -4.232 | 14.714 |
| ATOM | 1264 | C | LEU | B | 38 | 30.132 | -5.342 | 14.895 |
| ATOM | 1265 | O | LEU | B | 38 | 30.070 | -6.357 | 14.197 |
| ATOM | 1266 | CB | LEU | B | 38 | 27.986 | -4.237 | 15.802 |
| ATOM | 1267 | CG | LEU | B | 38 | 27.005 | -3.039 | 15.750 |
| ATOM | 1268 | CD1 | LEU | B | 38 | 25.885 | -3.214 | 16.788 |
| ATOM | 1269 | CD2 | LEU | B | 38 | 27.707 | -1.696 | 16.017 |
| ATOM | 1270 | N | PRO | B | 39 | 31.119 | -5.160 | 15.804 |
| ATOM | 1271 | CA | PRO | B | 39 | 32.199 | -6.116 | 16.052 |
| ATOM | 1272 | C | PRO | B | 39 | 31.767 | -7.223 | 17.028 |
| ATOM | 1273 | O | PRO | B | 39 | 31.448 | -6.942 | 18.185 |
| ATOM | 1274 | CB | PRO | B | 39 | 33.347 | -5.276 | 16.625 |
| ATOM | 1275 | CG | PRO | B | 39 | 32.634 | -4.148 | 17.370 |
| ATOM | 1276 | CD | PRO | B | 39 | 31.385 | -3.916 | 16.523 |
| ATOM | 1277 | N | GLY | B | 40 | 31.770 | -8.481 | 16.559 |
| ATOM | 1278 | H | GLY | B | 40 | 32.036 | -8.641 | 15.598 |
| ATOM | 1279 | CA | GLY | B | 40 | 31.420 | -9.658 | 17.353 |
| ATOM | 1280 | C | GLY | B | 40 | 30.679 | -10.723 | 16.539 |
| ATOM | 1281 | O | GLY | B | 40 | 30.647 | -10.671 | 15.308 |
| ATOM | 1282 | N | LYS | B | 41 | 30.098 | -11.699 | 17.255 |
| ATOM | 1283 | H | LYS | B | 41 | 30.164 | -11.656 | 18.261 |
| ATOM | 1284 | CA | LYS | B | 41 | 29.399 | -12.861 | 16.702 |
| ATOM | 1285 | C | LYS | B | 41 | 27.971 | -12.923 | 17.245 |
| ATOM | 1286 | O | LYS | B | 41 | 27.743 | -12.700 | 18.436 |

FIG. 11W

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1287 | CB | LYS | B | 41 | 30.154 | -14.152 | 17.048 |
| ATOM | 1288 | CG | LYS | B | 41 | 31.537 | -14.221 | 16.384 |
| ATOM | 1289 | CD | LYS | B | 41 | 32.192 | -15.580 | 16.651 |
| ATOM | 1290 | CE | LYS | B | 41 | 33.566 | -15.642 | 15.983 |
| ATOM | 1291 | NZ | LYS | B | 41 | 34.198 | -16.956 | 16.183 |
| ATOM | 1292 | 1HZ | LYS | B | 41 | 35.102 | -16.968 | 15.732 |
| ATOM | 1293 | 3HZ | LYS | B | 41 | 33.612 | -17.674 | 15.782 |
| ATOM | 1294 | 2HZ | LYS | B | 41 | 34.312 | -17.128 | 17.172 |
| ATOM | 1295 | N | TRP | B | 42 | 27.018 | -13.228 | 16.351 |
| ATOM | 1296 | H | TRP | B | 42 | 27.307 | -13.458 | 15.411 |
| ATOM | 1297 | CA | TRP | B | 42 | 25.597 | -12.929 | 16.521 |
| ATOM | 1298 | C | TRP | B | 42 | 24.723 | -14.179 | 16.405 |
| ATOM | 1299 | O | TRP | B | 42 | 25.210 | -15.277 | 16.131 |
| ATOM | 1300 | CB | TRP | B | 42 | 25.192 | -11.856 | 15.491 |
| ATOM | 1301 | CG | TRP | B | 42 | 26.127 | -10.687 | 15.390 |
| ATOM | 1302 | CD1 | TRP | B | 42 | 26.651 | -10.197 | 14.244 |
| ATOM | 1303 | CD2 | TRP | B | 42 | 26.739 | -9.913 | 16.467 |
| ATOM | 1304 | NE1 | TRP | B | 42 | 27.548 | -9.191 | 14.533 |
| ATOM | 1305 | HE1 | TRP | B | 42 | 28.067 | -8.702 | 13.818 |
| ATOM | 1306 | CE2 | TRP | B | 42 | 27.664 | -8.995 | 15.893 |
| ATOM | 1307 | CE3 | TRP | B | 42 | 26.640 | -9.923 | 17.875 |
| ATOM | 1308 | CZ2 | TRP | B | 42 | 28.443 | -8.136 | 16.680 |
| ATOM | 1309 | CZ3 | TRP | B | 42 | 27.426 | -9.075 | 18.673 |
| ATOM | 1310 | CH2 | TRP | B | 42 | 28.318 | -8.171 | 18.077 |
| ATOM | 1311 | N | LYS | B | 43 | 23.416 | -13.980 | 16.617 |
| ATOM | 1312 | H | LYS | B | 43 | 23.105 | -13.044 | 16.840 |
| ATOM | 1313 | CA | LYS | B | 43 | 22.378 | -14.995 | 16.526 |
| ATOM | 1314 | C | LYS | B | 43 | 21.368 | -14.507 | 15.478 |
| ATOM | 1315 | O | LYS | B | 43 | 20.743 | -13.472 | 15.706 |
| ATOM | 1316 | CB | LYS | B | 43 | 21.694 | -15.196 | 17.893 |
| ATOM | 1317 | CG | LYS | B | 43 | 22.641 | -15.623 | 19.034 |
| ATOM | 1318 | CD | LYS | B | 43 | 22.409 | -14.814 | 20.323 |
| ATOM | 1319 | CE | LYS | B | 43 | 22.767 | -13.327 | 20.182 |
| ATOM | 1320 | NZ | LYS | B | 43 | 24.214 | -13.113 | 20.015 |
| ATOM | 1321 | 1HZ | LYS | B | 43 | 24.400 | -12.125 | 19.924 |
| ATOM | 1322 | 3HZ | LYS | B | 43 | 24.532 | -13.593 | 19.185 |
| ATOM | 1323 | 2HZ | LYS | B | 43 | 24.702 | -13.476 | 20.821 |
| ATOM | 1324 | N | PRO | B | 44 | 21.175 | -15.204 | 14.341 |
| ATOM | 1325 | CA | PRO | B | 44 | 20.139 | -14.835 | 13.382 |
| ATOM | 1326 | C | PRO | B | 44 | 18.765 | -14.997 | 14.044 |
| ATOM | 1327 | O | PRO | B | 44 | 18.573 | -15.902 | 14.860 |
| ATOM | 1328 | CB | PRO | B | 44 | 20.341 | -15.761 | 12.180 |
| ATOM | 1329 | CG | PRO | B | 44 | 20.999 | -16.999 | 12.787 |
| ATOM | 1330 | CD | PRO | B | 44 | 21.837 | -16.434 | 13.933 |
| ATOM | 1331 | N | LYS | B | 45 | 17.825 | -14.101 | 13.712 |
| ATOM | 1332 | H | LYS | B | 45 | 17.994 | -13.483 | 12.944 |
| ATOM | 1333 | CA | LYS | B | 45 | 16.523 | -14.088 | 14.339 |
| ATOM | 1334 | C | LYS | B | 45 | 15.519 | -13.590 | 13.329 |
| ATOM | 1335 | O | LYS | B | 45 | 15.829 | -12.838 | 12.379 |
| ATOM | 1336 | CB | LYS | B | 45 | 16.558 | -13.149 | 15.560 |
| ATOM | 1337 | CG | LYS | B | 45 | 15.469 | -13.442 | 16.579 |
| ATOM | 1338 | CD | LYS | B | 45 | 15.256 | -12.254 | 17.501 |
| ATOM | 1339 | CE | LYS | B | 45 | 14.131 | -12.461 | 18.469 |
| ATOM | 1340 | NZ | LYS | B | 45 | 14.549 | -13.442 | 19.474 |
| ATOM | 1341 | 1HZ | LYS | B | 45 | 13.805 | -13.588 | 20.126 |
| ATOM | 1342 | 3HZ | LYS | B | 45 | 15.355 | -13.101 | 19.958 |

FIG. 1IX

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1343 | 2HZ | LYS | B | 45 | 14.772 | -14.306 | 19.023 |
| ATOM | 1344 | N | MET | B | 46 | 14.240 | -14.005 | 13.416 |
| ATOM | 1345 | H | MET | B | 46 | 13.991 | -14.705 | 14.085 |
| ATOM | 1346 | CA | MET | B | 46 | 13.203 | -13.472 | 12.570 |
| ATOM | 1347 | C | MET | B | 46 | 12.291 | -12.623 | 13.425 |
| ATOM | 1348 | O | MET | B | 46 | 11.782 | -13.063 | 14.471 |
| ATOM | 1349 | CB | MET | B | 46 | 12.383 | -14.616 | 12.016 |
| ATOM | 1350 | CG | MET | B | 46 | 13.153 | -15.586 | 11.187 |
| ATOM | 1351 | SD | MET | B | 46 | 12.977 | -15.188 | 9.473 |
| ATOM | 1352 | CE | MET | B | 46 | 13.566 | -16.690 | 8.775 |
| ATOM | 1353 | N | ILE | B | 47 | 11.933 | -11.379 | 13.030 |
| ATOM | 1354 | H | ILE | B | 47 | 12.327 | -10.991 | 12.196 |
| ATOM | 1355 | CA | ILE | B | 47 | 10.971 | -10.568 | 13.797 |
| ATOM | 1356 | C | ILE | B | 47 | 9.761 | -10.233 | 12.962 |
| ATOM | 1357 | O | ILE | B | 47 | 9.819 | -10.048 | 11.731 |
| ATOM | 1358 | CB | ILE | B | 47 | 11.608 | -9.294 | 14.385 |
| ATOM | 1359 | CG1 | ILE | B | 47 | 12.345 | -8.459 | 13.318 |
| ATOM | 1360 | CG2 | ILE | B | 47 | 12.542 | -9.638 | 15.494 |
| ATOM | 1361 | CD1 | ILE | B | 47 | 12.789 | -7.123 | 13.851 |
| ATOM | 1362 | N | GLY | B | 48 | 8.557 | -10.136 | 13.558 |
| ATOM | 1363 | H | GLY | B | 48 | 8.484 | -10.249 | 14.549 |
| ATOM | 1364 | CA | GLY | B | 48 | 7.365 | -9.872 | 12.800 |
| ATOM | 1365 | C | GLY | B | 48 | 6.826 | -8.512 | 13.141 |
| ATOM | 1366 | O | GLY | B | 48 | 7.136 | -7.832 | 14.149 |
| ATOM | 1367 | N | GLY | B | 49 | 5.940 | -8.027 | 12.306 |
| ATOM | 1368 | H | GLY | B | 49 | 5.668 | -8.562 | 11.506 |
| ATOM | 1369 | CA | GLY | B | 49 | 5.336 | -6.745 | 12.493 |
| ATOM | 1370 | C | GLY | B | 49 | 4.082 | -6.786 | 11.674 |
| ATOM | 1371 | O | GLY | B | 49 | 3.561 | -7.847 | 11.273 |
| ATOM | 1372 | N | ILE | B | 50 | 3.531 | -5.634 | 11.315 |
| ATOM | 1373 | H | ILE | B | 50 | 4.015 | -4.777 | 11.492 |
| ATOM | 1374 | CA | ILE | B | 50 | 2.247 | -5.573 | 10.673 |
| ATOM | 1375 | C | ILE | B | 50 | 2.118 | -6.456 | 9.420 |
| ATOM | 1376 | O | ILE | B | 50 | 1.175 | -7.253 | 9.215 |
| ATOM | 1377 | CB | ILE | B | 50 | 1.982 | -4.071 | 10.391 |
| ATOM | 1378 | CG1 | ILE | B | 50 | 1.005 | -3.539 | 11.396 |
| ATOM | 1379 | CG2 | ILE | B | 50 | 1.610 | -3.739 | 8.922 |
| ATOM | 1380 | CD1 | ILE | B | 50 | -0.391 | -4.077 | 11.252 |
| ATOM | 1381 | N | GLY | B | 51 | 3.113 | -6.410 | 8.519 |
| ATOM | 1382 | H | GLY | B | 51 | 3.957 | -5.920 | 8.737 |
| ATOM | 1383 | CA | GLY | B | 51 | 2.926 | -7.075 | 7.259 |
| ATOM | 1384 | C | GLY | B | 51 | 3.671 | -8.391 | 7.077 |
| ATOM | 1385 | O | GLY | B | 51 | 3.716 | -8.945 | 5.973 |
| ATOM | 1386 | N | GLY | B | 52 | 4.296 | -8.982 | 8.116 |
| ATOM | 1387 | H | GLY | B | 52 | 4.227 | -8.580 | 9.029 |
| ATOM | 1388 | CA | GLY | B | 52 | 5.053 | -10.190 | 7.874 |
| ATOM | 1389 | C | GLY | B | 52 | 6.334 | -10.178 | 8.678 |
| ATOM | 1390 | O | GLY | B | 52 | 6.519 | -9.421 | 9.657 |
| ATOM | 1391 | N | PHE | B | 53 | 7.325 | -11.015 | 8.343 |
| ATOM | 1392 | H | PHE | B | 53 | 7.227 | -11.603 | 7.540 |
| ATOM | 1393 | CA | PHE | B | 53 | 8.542 | -11.096 | 9.110 |
| ATOM | 1394 | C | PHE | B | 53 | 9.727 | -10.584 | 8.315 |
| ATOM | 1395 | O | PHE | B | 53 | 9.780 | -10.618 | 7.075 |
| ATOM | 1396 | CB | PHE | B | 53 | 8.804 | -12.555 | 9.542 |
| ATOM | 1397 | CG | PHE | B | 53 | 7.850 | -13.023 | 10.592 |
| ATOM | 1398 | CD1 | PHE | B | 53 | 6.513 | -13.277 | 10.279 |

FIG. 11Y

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1399 | CD2 | PHE | B | 53 | 8.279 | -13.192 | 11.918 |
| ATOM | 1400 | CE1 | PHE | B | 53 | 5.620 | -13.697 | 11.253 |
| ATOM | 1401 | CE2 | PHE | B | 53 | 7.382 | -13.615 | 12.903 |
| ATOM | 1402 | CZ | PHE | B | 53 | 6.052 | -13.868 | 12.574 |
| ATOM | 1403 | N | ILE | B | 54 | 10.758 | -10.126 | 8.985 |
| ATOM | 1404 | H | ILE | B | 54 | 10.665 | -9.922 | 9.960 |
| ATOM | 1405 | CA | ILE | B | 54 | 12.029 | -9.910 | 8.338 |
| ATOM | 1406 | C | ILE | B | 54 | 13.089 | -10.648 | 9.134 |
| ATOM | 1407 | O | ILE | B | 54 | 12.952 | -11.006 | 10.325 |
| ATOM | 1408 | CB | ILE | B | 54 | 12.390 | -8.444 | 8.236 |
| ATOM | 1409 | CG1 | ILE | B | 54 | 12.386 | -7.775 | 9.611 |
| ATOM | 1410 | CG2 | ILE | B | 54 | 11.460 | -7.770 | 7.218 |
| ATOM | 1411 | CD1 | ILE | B | 54 | 13.113 | -6.438 | 9.590 |
| ATOM | 1412 | N | LYS | B | 55 | 14.272 | -10.852 | 8.523 |
| ATOM | 1413 | H | LYS | B | 55 | 14.383 | -10.599 | 7.562 |
| ATOM | 1414 | CA | LYS | B | 55 | 15.403 | -11.431 | 9.216 |
| ATOM | 1415 | C | LYS | B | 55 | 16.274 | -10.324 | 9.732 |
| ATOM | 1416 | O | LYS | B | 55 | 16.620 | -9.328 | 9.047 |
| ATOM | 1417 | CB | LYS | B | 55 | 16.222 | -12.237 | 8.245 |
| ATOM | 1418 | CG | LYS | B | 55 | 15.638 | -13.596 | 8.063 |
| ATOM | 1419 | CD | LYS | B | 55 | 16.299 | -14.348 | 6.953 |
| ATOM | 1420 | CE | LYS | B | 55 | 15.311 | -14.520 | 5.813 |
| ATOM | 1421 | NZ | LYS | B | 55 | 15.757 | -15.577 | 4.897 |
| ATOM | 1422 | 1HZ | LYS | B | 55 | 15.095 | -15.676 | 4.154 |
| ATOM | 1423 | 3HZ | LYS | B | 55 | 15.830 | -16.441 | 5.395 |
| ATOM | 1424 | 2HZ | LYS | B | 55 | 16.650 | -15.334 | 4.518 |
| ATOM | 1425 | N | VAL | B | 56 | 16.880 | -10.547 | 10.910 |
| ATOM | 1426 | H | VAL | B | 56 | 16.741 | -11.418 | 11.382 |
| ATOM | 1427 | CA | VAL | B | 56 | 17.732 | -9.578 | 11.534 |
| ATOM | 1428 | C | VAL | B | 56 | 18.884 | -10.304 | 12.184 |
| ATOM | 1429 | O | VAL | B | 56 | 18.884 | -11.539 | 12.367 |
| ATOM | 1430 | CB | VAL | B | 56 | 16.912 | -8.819 | 12.609 |
| ATOM | 1431 | CG1 | VAL | B | 56 | 15.865 | -7.943 | 11.921 |
| ATOM | 1432 | CG2 | VAL | B | 56 | 16.215 | -9.788 | 13.599 |
| ATOM | 1433 | N | ARG | B | 57 | 19.958 | -9.593 | 12.591 |
| ATOM | 1434 | H | ARG | B | 57 | 20.030 | -8.624 | 12.353 |
| ATOM | 1435 | CA | ARG | B | 57 | 21.050 | -10.193 | 13.386 |
| ATOM | 1436 | C | ARG | B | 57 | 20.963 | -9.608 | 14.804 |
| ATOM | 1437 | O | ARG | B | 57 | 20.814 | -8.395 | 15.053 |
| ATOM | 1438 | CB | ARG | B | 57 | 22.426 | -9.873 | 12.817 |
| ATOM | 1439 | CG | ARG | B | 57 | 22.664 | -10.437 | 11.439 |
| ATOM | 1440 | CD | ARG | B | 57 | 24.012 | -10.065 | 10.899 |
| ATOM | 1441 | NE | ARG | B | 57 | 24.280 | -10.697 | 9.617 |
| ATOM | 1442 | HE | ARG | B | 57 | 23.592 | -11.323 | 9.250 |
| ATOM | 1443 | CZ | ARG | B | 57 | 25.392 | -10.478 | 8.921 |
| ATOM | 1444 | NH1 | ARG | B | 57 | 26.337 | -9.650 | 9.353 |
| ATOM | 1445 | 2HH1 | ARG | B | 57 | 26.223 | -9.171 | 10.224 |
| ATOM | 1446 | 1HH1 | ARG | B | 57 | 27.163 | -9.505 | 8.808 |
| ATOM | 1447 | NH2 | ARG | B | 57 | 25.561 | -11.104 | 7.760 |
| ATOM | 1448 | 1HH2 | ARG | B | 57 | 26.392 | -10.950 | 7.225 |
| ATOM | 1449 | 2HH2 | ARG | B | 57 | 24.857 | -11.729 | 7.422 |
| ATOM | 1450 | N | GLN | B | 58 | 20.997 | -10.489 | 15.832 |
| ATOM | 1451 | H | GLN | B | 58 | 21.176 | -11.456 | 15.650 |
| ATOM | 1452 | CA | GLN | B | 58 | 20.780 | -10.072 | 17.206 |
| ATOM | 1453 | C | GLN | B | 58 | 22.108 | -9.886 | 17.882 |
| ATOM | 1454 | O | GLN | B | 58 | 22.918 | -10.815 | 18.038 |

FIG. 11Z

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1455 | CB | GLN | B | 58 | 20.051 | -11.190 | 17.932 |
| ATOM | 1456 | CG | GLN | B | 58 | 19.765 | -10.845 | 19.366 |
| ATOM | 1457 | CD | GLN | B | 58 | 19.179 | -12.003 | 20.112 |
| ATOM | 1458 | OE1 | GLN | B | 58 | 19.712 | -12.472 | 21.101 |
| ATOM | 1459 | NE2 | GLN | B | 58 | 18.055 | -12.476 | 19.623 |
| ATOM | 1460 | 1HE2 | GLN | B | 58 | 17.598 | -13.249 | 20.063 |
| ATOM | 1461 | 2HE2 | GLN | B | 58 | 17.647 | -12.066 | 18.807 |
| ATOM | 1462 | N | TYR | B | 59 | 22.416 | -8.692 | 18.422 |
| ATOM | 1463 | H | TYR | B | 59 | 21.788 | -7.921 | 18.311 |
| ATOM | 1464 | CA | TYR | B | 59 | 23.631 | -8.486 | 19.161 |
| ATOM | 1465 | C | TYR | B | 59 | 23.244 | -8.290 | 20.607 |
| ATOM | 1466 | O | TYR | B | 59 | 22.178 | -7.728 | 20.927 |
| ATOM | 1467 | CB | TYR | B | 59 | 24.387 | -7.241 | 18.653 |
| ATOM | 1468 | CG | TYR | B | 59 | 24.271 | -7.075 | 17.149 |
| ATOM | 1469 | CD1 | TYR | B | 59 | 23.045 | -7.242 | 16.494 |
| ATOM | 1470 | CD2 | TYR | B | 59 | 25.385 | -6.753 | 16.374 |
| ATOM | 1471 | CE1 | TYR | B | 59 | 22.939 | -7.093 | 15.112 |
| ATOM | 1472 | CE2 | TYR | B | 59 | 25.291 | -6.603 | 14.995 |
| ATOM | 1473 | CZ | TYR | B | 59 | 24.068 | -6.774 | 14.365 |
| ATOM | 1474 | OH | TYR | B | 59 | 24.018 | -6.620 | 13.010 |
| ATOM | 1475 | HH | TYR | B | 59 | 24.926 | -6.394 | 12.658 |
| ATOM | 1476 | N | ASP | B | 60 | 24.010 | -8.785 | 21.596 |
| ATOM | 1477 | H | ASP | B | 60 | 24.852 | -9.276 | 21.372 |
| ATOM | 1478 | CA | ASP | B | 60 | 23.644 | -8.624 | 22.992 |
| ATOM | 1479 | C | ASP | B | 60 | 24.556 | -7.595 | 23.615 |
| ATOM | 1480 | O | ASP | B | 60 | 25.654 | -7.261 | 23.125 |
| ATOM | 1481 | CB | ASP | B | 60 | 23.789 | -9.920 | 23.777 |
| ATOM | 1482 | CG | ASP | B | 60 | 22.803 | -10.960 | 23.332 |
| ATOM | 1483 | OD1 | ASP | B | 60 | 21.619 | -10.634 | 23.032 |
| ATOM | 1484 | OD2 | ASP | B | 60 | 23.208 | -12.126 | 23.273 |
| ATOM | 1485 | N | GLN | B | 61 | 24.156 | -7.022 | 24.774 |
| ATOM | 1486 | H | GLN | B | 61 | 23.252 | -7.234 | 25.146 |
| ATOM | 1487 | CA | GLN | B | 61 | 25.011 | -6.086 | 25.519 |
| ATOM | 1488 | C | GLN | B | 61 | 25.411 | -4.866 | 24.746 |
| ATOM | 1489 | O | GLN | B | 61 | 26.560 | -4.382 | 24.832 |
| ATOM | 1490 | CB | GLN | B | 61 | 26.269 | -6.763 | 26.028 |
| ATOM | 1491 | CG | GLN | B | 61 | 26.020 | -8.038 | 26.753 |
| ATOM | 1492 | CD | GLN | B | 61 | 25.714 | -7.766 | 28.185 |
| ATOM | 1493 | OE1 | GLN | B | 61 | 24.572 | -7.455 | 28.548 |
| ATOM | 1494 | NE2 | GLN | B | 61 | 26.744 | -7.844 | 29.014 |
| ATOM | 1495 | 1HE2 | GLN | B | 61 | 26.620 | -7.675 | 29.992 |
| ATOM | 1496 | 2HE2 | GLN | B | 61 | 27.654 | -8.073 | 28.669 |
| ATOM | 1497 | N | ILE | B | 62 | 24.539 | -4.257 | 23.933 |
| ATOM | 1498 | H | ILE | B | 62 | 23.628 | -4.648 | 23.801 |
| ATOM | 1499 | CA | ILE | B | 62 | 24.878 | -3.047 | 23.238 |
| ATOM | 1500 | C | ILE | B | 62 | 24.571 | -1.885 | 24.144 |
| ATOM | 1501 | O | ILE | B | 62 | 23.515 | -1.819 | 24.819 |
| ATOM | 1502 | CB | ILE | B | 62 | 24.097 | -2.922 | 21.912 |
| ATOM | 1503 | CG1 | ILE | B | 62 | 24.310 | -4.170 | 21.094 |
| ATOM | 1504 | CG2 | ILE | B | 62 | 24.568 | -1.709 | 21.067 |
| ATOM | 1505 | CD1 | ILE | B | 62 | 25.794 | -4.479 | 20.878 |
| ATOM | 1506 | N | LEU | B | 63 | 25.485 | -0.912 | 24.304 |
| ATOM | 1507 | H | LEU | B | 63 | 26.403 | -1.028 | 23.926 |
| ATOM | 1508 | CA | LEU | B | 63 | 25.192 | 0.322 | 25.015 |
| ATOM | 1509 | C | LEU | B | 63 | 24.630 | 1.296 | 24.030 |
| ATOM | 1510 | O | LEU | B | 63 | 25.239 | 1.658 | 22.995 |

FIG. 1 laa

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1511 | CB | LEU | B | 63 | 26.436 | 0.970 | 25.590 |
| ATOM | 1512 | CG | LEU | B | 63 | 26.186 | 2.358 | 26.226 |
| ATOM | 1513 | CD1 | LEU | B | 63 | 25.486 | 2.261 | 27.576 |
| ATOM | 1514 | CD2 | LEU | B | 63 | 27.468 | 3.162 | 26.382 |
| ATOM | 1515 | N | ILE | B | 64 | 23.492 | 1.946 | 24.358 |
| ATOM | 1516 | H | ILE | B | 64 | 22.958 | 1.643 | 25.148 |
| ATOM | 1517 | CA | ILE | B | 64 | 23.003 | 3.068 | 23.617 |
| ATOM | 1518 | C | ILE | B | 64 | 22.872 | 4.194 | 24.612 |
| ATOM | 1519 | O | ILE | B | 64 | 22.915 | 4.007 | 25.846 |
| ATOM | 1520 | CB | ILE | B | 64 | 21.634 | 2.701 | 22.989 |
| ATOM | 1521 | CG1 | ILE | B | 64 | 21.825 | 1.521 | 22.029 |
| ATOM | 1522 | CG2 | ILE | B | 64 | 20.982 | 3.894 | 22.246 |
| ATOM | 1523 | CD1 | ILE | B | 64 | 20.593 | 1.096 | 21.260 |
| ATOM | 1524 | N | GLU | B | 65 | 22.803 | 5.460 | 24.172 |
| ATOM | 1525 | H | GLU | B | 65 | 23.013 | 5.664 | 23.216 |
| ATOM | 1526 | CA | GLU | B | 65 | 22.432 | 6.551 | 25.037 |
| ATOM | 1527 | C | GLU | B | 65 | 21.242 | 7.194 | 24.373 |
| ATOM | 1528 | O | GLU | B | 65 | 21.312 | 7.729 | 23.257 |
| ATOM | 1529 | CB | GLU | B | 65 | 23.497 | 7.615 | 25.131 |
| ATOM | 1530 | CG | GLU | B | 65 | 24.787 | 7.196 | 25.761 |
| ATOM | 1531 | CD | GLU | B | 65 | 25.694 | 8.385 | 26.076 |
| ATOM | 1532 | OE1 | GLU | B | 65 | 25.170 | 9.510 | 26.311 |
| ATOM | 1533 | OE2 | GLU | B | 65 | 26.938 | 8.200 | 26.092 |
| ATOM | 1534 | N | ILE | B | 66 | 20.078 | 7.240 | 25.035 |
| ATOM | 1535 | H | ILE | B | 66 | 20.010 | 6.835 | 25.947 |
| ATOM | 1536 | CA | ILE | B | 66 | 18.907 | 7.865 | 24.462 |
| ATOM | 1537 | C | ILE | B | 66 | 18.777 | 9.195 | 25.145 |
| ATOM | 1538 | O | ILE | B | 66 | 18.591 | 9.303 | 26.379 |
| ATOM | 1539 | CB | ILE | B | 66 | 17.713 | 6.995 | 24.790 |
| ATOM | 1540 | CG1 | ILE | B | 66 | 17.916 | 5.583 | 24.335 |
| ATOM | 1541 | CG2 | ILE | B | 66 | 16.405 | 7.544 | 24.177 |
| ATOM | 1542 | CD1 | ILE | B | 66 | 16.888 | 4.677 | 24.884 |
| ATOM | 1543 | N | CYS | B | 67 | 18.965 | 10.325 | 24.437 |
| ATOM | 1544 | H | CYS | B | 67 | 19.201 | 10.268 | 23.467 |
| ATOM | 1545 | CA | CYS | B | 67 | 18.833 | 11.663 | 25.049 |
| ATOM | 1546 | C | CYS | B | 67 | 19.637 | 11.781 | 26.319 |
| ATOM | 1547 | O | CYS | B | 67 | 19.235 | 12.400 | 27.328 |
| ATOM | 1548 | CB | CYS | B | 67 | 17.387 | 12.023 | 25.319 |
| ATOM | 1549 | SG | CYS | B | 67 | 16.407 | 12.259 | 23.821 |
| ATOM | 1550 | N | GLY | B | 68 | 20.830 | 11.180 | 26.383 |
| ATOM | 1551 | H | GLY | B | 68 | 21.158 | 10.646 | 25.604 |
| ATOM | 1552 | CA | GLY | B | 68 | 21.654 | 11.288 | 27.558 |
| ATOM | 1553 | C | GLY | B | 68 | 21.464 | 10.185 | 28.584 |
| ATOM | 1554 | O | GLY | B | 68 | 22.174 | 10.128 | 29.606 |
| ATOM | 1555 | N | HIS | B | 69 | 20.513 | 9.255 | 28.425 |
| ATOM | 1556 | H | HIS | B | 69 | 19.924 | 9.282 | 27.618 |
| ATOM | 1557 | CA | HIS | B | 69 | 20.304 | 8.199 | 29.391 |
| ATOM | 1558 | C | HIS | B | 69 | 20.861 | 6.936 | 28.811 |
| ATOM | 1559 | O | HIS | B | 69 | 20.589 | 6.560 | 27.647 |
| ATOM | 1560 | CB | HIS | B | 69 | 18.832 | 7.992 | 29.654 |
| ATOM | 1561 | CG | HIS | B | 69 | 18.175 | 9.203 | 30.223 |
| ATOM | 1562 | ND1 | HIS | B | 69 | 17.504 | 9.195 | 31.435 |
| ATOM | 1563 | HD1 | HIS | B | 69 | 17.383 | 8.402 | 32.032 |
| ATOM | 1564 | CD2 | HIS | B | 69 | 18.122 | 10.470 | 29.729 |
| ATOM | 1565 | CE1 | HIS | B | 69 | 17.070 | 10.429 | 31.626 |
| ATOM | 1566 | NE2 | HIS | B | 69 | 17.410 | 11.240 | 30.635 |

FIG. 1bb

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1567 | N | LYS | B | 70 | 21.751 | 6.217 | 29.499 |
| ATOM | 1568 | H | LYS | B | 70 | 22.025 | 6.512 | 30.414 |
| ATOM | 1569 | CA | LYS | B | 70 | 22.326 | 5.020 | 28.945 |
| ATOM | 1570 | C | LYS | B | 70 | 21.386 | 3.854 | 29.145 |
| ATOM | 1571 | O | LYS | B | 70 | 20.627 | 3.725 | 30.120 |
| ATOM | 1572 | CB | LYS | B | 70 | 23.613 | 4.678 | 29.663 |
| ATOM | 1573 | CG | LYS | B | 70 | 24.694 | 5.655 | 29.379 |
| ATOM | 1574 | CD | LYS | B | 70 | 25.739 | 5.524 | 30.444 |
| ATOM | 1575 | CE | LYS | B | 70 | 27.048 | 6.090 | 30.011 |
| ATOM | 1576 | NZ | LYS | B | 70 | 26.948 | 7.548 | 30.000 |
| ATOM | 1577 | 1HZ | LYS | B | 70 | 27.821 | 7.940 | 29.711 |
| ATOM | 1578 | 3HZ | LYS | B | 70 | 26.725 | 7.874 | 30.919 |
| ATOM | 1579 | 2HZ | LYS | B | 70 | 26.230 | 7.828 | 29.363 |
| ATOM | 1580 | N | ALA | B | 71 | 21.512 | 2.849 | 28.284 |
| ATOM | 1581 | H | ALA | B | 71 | 22.141 | 2.934 | 27.512 |
| ATOM | 1582 | CA | ALA | B | 71 | 20.762 | 1.630 | 28.432 |
| ATOM | 1583 | C | ALA | B | 71 | 21.629 | 0.576 | 27.805 |
| ATOM | 1584 | O | ALA | B | 71 | 22.463 | 0.830 | 26.912 |
| ATOM | 1585 | CB | ALA | B | 71 | 19.452 | 1.726 | 27.737 |
| ATOM | 1586 | N | ILE | B | 72 | 21.547 | -0.681 | 28.237 |
| ATOM | 1587 | H | ILE | B | 72 | 20.864 | -0.925 | 28.926 |
| ATOM | 1588 | CA | ILE | B | 72 | 22.424 | -1.698 | 27.730 |
| ATOM | 1589 | C | ILE | B | 72 | 21.615 | -2.938 | 27.462 |
| ATOM | 1590 | O | ILE | B | 72 | 20.909 | -3.490 | 28.330 |
| ATOM | 1591 | CB | ILE | B | 72 | 23.524 | -1.999 | 28.737 |
| ATOM | 1592 | CG1 | ILE | B | 72 | 24.322 | -0.735 | 29.090 |
| ATOM | 1593 | CG2 | ILE | B | 72 | 24.442 | -3.037 | 28.153 |
| ATOM | 1594 | CD1 | ILE | B | 72 | 25.374 | -1.012 | 30.163 |
| ATOM | 1595 | N | GLY | B | 73 | 21.609 | -3.446 | 26.235 |
| ATOM | 1596 | H | GLY | B | 73 | 22.204 | -3.054 | 25.534 |
| ATOM | 1597 | CA | GLY | B | 73 | 20.707 | -4.545 | 26.062 |
| ATOM | 1598 | C | GLY | B | 73 | 20.828 | -5.084 | 24.663 |
| ATOM | 1599 | O | GLY | B | 73 | 21.754 | -4.831 | 23.863 |
| ATOM | 1600 | N | THR | B | 74 | 19.856 | -5.905 | 24.271 |
| ATOM | 1601 | H | THR | B | 74 | 19.086 | -6.088 | 24.882 |
| ATOM | 1602 | CA | THR | B | 74 | 19.869 | -6.548 | 22.988 |
| ATOM | 1603 | C | THR | B | 74 | 19.363 | -5.590 | 21.931 |
| ATOM | 1604 | O | THR | B | 74 | 18.338 | -4.870 | 22.053 |
| ATOM | 1605 | CB | THR | B | 74 | 19.011 | -7.801 | 23.074 |
| ATOM | 1606 | OG1 | THR | B | 74 | 19.611 | -8.683 | 24.013 |
| ATOM | 1607 | HG1 | THR | B | 74 | 19.068 | -9.519 | 24.092 |
| ATOM | 1608 | CG2 | THR | B | 74 | 18.817 | -8.496 | 21.705 |
| ATOM | 1609 | N | VAL | B | 75 | 20.028 | -5.620 | 20.762 |
| ATOM | 1610 | H | VAL | B | 75 | 20.835 | -6.203 | 20.666 |
| ATOM | 1611 | CA | VAL | B | 75 | 19.630 | -4.837 | 19.611 |
| ATOM | 1612 | C | VAL | B | 75 | 19.600 | -5.771 | 18.426 |
| ATOM | 1613 | O | VAL | B | 75 | 20.444 | -6.673 | 18.230 |
| ATOM | 1614 | CB | VAL | B | 75 | 20.667 | -3.712 | 19.395 |
| ATOM | 1615 | CG1 | VAL | B | 75 | 20.473 | -3.002 | 18.046 |
| ATOM | 1616 | CG2 | VAL | B | 75 | 20.679 | -2.708 | 20.567 |
| ATOM | 1617 | N | LEU | B | 76 | 18.557 | -5.647 | 17.565 |
| ATOM | 1618 | H | LEU | B | 76 | 17.822 | -5.000 | 17.767 |
| ATOM | 1619 | CA | LEU | B | 76 | 18.444 | -6.427 | 16.324 |
| ATOM | 1620 | C | LEU | B | 76 | 18.736 | -5.487 | 15.144 |
| ATOM | 1621 | O | LEU | B | 76 | 18.239 | -4.343 | 15.040 |
| ATOM | 1622 | CB | LEU | B | 76 | 17.028 | -7.021 | 16.158 |

FIG. 11cc

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1623 | CG | LEU | B | 76 | 16.427 | -7.612 | 17.449 |
| ATOM | 1624 | CD1 | LEU | B | 76 | 14.992 | -8.075 | 17.263 |
| ATOM | 1625 | CD2 | LEU | B | 76 | 17.266 | -8.758 | 18.019 |
| ATOM | 1626 | N | VAL | B | 77 | 19.607 | -5.900 | 14.222 |
| ATOM | 1627 | H | VAL | B | 77 | 19.985 | -6.824 | 14.276 |
| ATOM | 1628 | CA | VAL | B | 77 | 20.027 | -5.042 | 13.133 |
| ATOM | 1629 | C | VAL | B | 77 | 19.570 | -5.662 | 11.842 |
| ATOM | 1630 | O | VAL | B | 77 | 19.678 | -6.883 | 11.598 |
| ATOM | 1631 | CB | VAL | B | 77 | 21.563 | -4.905 | 13.191 |
| ATOM | 1632 | CG1 | VAL | B | 77 | 22.129 | -4.202 | 11.944 |
| ATOM | 1633 | CG2 | VAL | B | 77 | 22.030 | -4.166 | 14.470 |
| ATOM | 1634 | N | GLY | B | 78 | 18.978 | -4.915 | 10.943 |
| ATOM | 1635 | H | GLY | B | 78 | 18.841 | -3.941 | 11.121 |
| ATOM | 1636 | CA | GLY | B | 78 | 18.523 | -5.475 | 9.705 |
| ATOM | 1637 | C | GLY | B | 78 | 18.019 | -4.338 | 8.874 |
| ATOM | 1638 | O | GLY | B | 78 | 18.130 | -3.142 | 9.223 |
| ATOM | 1639 | N | PRO | B | 79 | 17.408 | -4.596 | 7.722 |
| ATOM | 1640 | CA | PRO | B | 79 | 16.954 | -3.535 | 6.834 |
| ATOM | 1641 | C | PRO | B | 79 | 15.635 | -2.872 | 7.280 |
| ATOM | 1642 | O | PRO | B | 79 | 14.609 | -2.877 | 6.565 |
| ATOM | 1643 | CB | PRO | B | 79 | 16.804 | -4.274 | 5.492 |
| ATOM | 1644 | CG | PRO | B | 79 | 16.463 | -5.712 | 5.881 |
| ATOM | 1645 | CD | PRO | B | 79 | 17.159 | -5.959 | 7.189 |
| ATOM | 1646 | N | THR | B | 80 | 15.574 | -2.247 | 8.458 |
| ATOM | 1647 | H | THR | B | 80 | 16.374 | -2.242 | 9.058 |
| ATOM | 1648 | CA | THR | B | 80 | 14.364 | -1.583 | 8.865 |
| ATOM | 1649 | C | THR | B | 80 | 14.312 | -0.189 | 8.228 |
| ATOM | 1650 | O | THR | B | 80 | 15.349 | 0.471 | 8.001 |
| ATOM | 1651 | CB | THR | B | 80 | 14.250 | -1.512 | 10.410 |
| ATOM | 1652 | OG1 | THR | B | 80 | 13.079 | -0.802 | 10.806 |
| ATOM | 1653 | HG1 | THR | B | 80 | 13.022 | -0.766 | 11.804 |
| ATOM | 1654 | CG2 | THR | B | 80 | 15.519 | -0.901 | 11.062 |
| ATOM | 1655 | N | PRO | B | 81 | 13.137 | 0.354 | 7.885 |
| ATOM | 1656 | CA | PRO | B | 81 | 13.036 | 1.747 | 7.379 |
| ATOM | 1657 | C | PRO | B | 81 | 13.363 | 2.732 | 8.484 |
| ATOM | 1658 | O | PRO | B | 81 | 13.791 | 3.880 | 8.250 |
| ATOM | 1659 | CB | PRO | B | 81 | 11.548 | 1.912 | 6.982 |
| ATOM | 1660 | CG | PRO | B | 81 | 10.819 | 0.674 | 7.488 |
| ATOM | 1661 | CD | PRO | B | 81 | 11.854 | -0.387 | 7.797 |
| ATOM | 1662 | N | VAL | B | 82 | 13.197 | 2.368 | 9.772 |
| ATOM | 1663 | H | VAL | B | 82 | 12.940 | 1.427 | 9.992 |
| ATOM | 1664 | CA | VAL | B | 82 | 13.380 | 3.306 | 10.885 |
| ATOM | 1665 | C | VAL | B | 82 | 14.160 | 2.668 | 12.010 |
| ATOM | 1666 | O | VAL | B | 82 | 14.045 | 1.465 | 12.293 |
| ATOM | 1667 | CB | VAL | B | 82 | 11.996 | 3.695 | 11.431 |
| ATOM | 1668 | CG1 | VAL | B | 82 | 12.055 | 4.961 | 12.269 |
| ATOM | 1669 | CG2 | VAL | B | 82 | 10.958 | 3.857 | 10.318 |
| ATOM | 1670 | N | ASN | B | 83 | 14.963 | 3.422 | 12.775 |
| ATOM | 1671 | H | ASN | B | 83 | 15.147 | 4.370 | 12.516 |
| ATOM | 1672 | CA | ASN | B | 83 | 15.550 | 2.846 | 13.967 |
| ATOM | 1673 | C | ASN | B | 83 | 14.481 | 2.874 | 15.022 |
| ATOM | 1674 | O | ASN | B | 83 | 13.814 | 3.903 | 15.294 |
| ATOM | 1675 | CB | ASN | B | 83 | 16.743 | 3.639 | 14.472 |
| ATOM | 1676 | CG | ASN | B | 83 | 17.935 | 3.574 | 13.570 |
| ATOM | 1677 | OD1 | ASN | B | 83 | 18.409 | 2.511 | 13.167 |
| ATOM | 1678 | ND2 | ASN | B | 83 | 18.439 | 4.735 | 13.238 |

FIG. 1 ldd

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ATOM | 1679 | 2HD2 | ASN | B | 83 | 19.237 | 4.786 | 12.638 |
| ATOM | 1680 | 1HD2 | ASN | B | 83 | 18.030 | 5.580 | 13.582 |
| ATOM | 1681 | N | ILE | B | 84 | 14.225 | 1.749 | 15.711 |
| ATOM | 1682 | H | ILE | B | 84 | 14.791 | 0.938 | 15.564 |
| ATOM | 1683 | CA | ILE | B | 84 | 13.154 | 1.658 | 16.667 |
| ATOM | 1684 | C | ILE | B | 84 | 13.740 | 1.317 | 18.020 |
| ATOM | 1685 | O | ILE | B | 84 | 14.428 | 0.300 | 18.223 |
| ATOM | 1686 | CB | ILE | B | 84 | 12.214 | 0.517 | 16.260 |
| ATOM | 1687 | CG1 | ILE | B | 84 | 11.656 | 0.759 | 14.849 |
| ATOM | 1688 | CG2 | ILE | B | 84 | 11.128 | 0.247 | 17.315 |
| ATOM | 1689 | CD1 | ILE | B | 84 | 10.770 | -0.359 | 14.291 |
| ATOM | 1690 | N | ILE | B | 85 | 13.483 | 2.157 | 19.051 |
| ATOM | 1691 | H | ILE | B | 85 | 13.028 | 3.030 | 18.877 |
| ATOM | 1692 | CA | ILE | B | 85 | 13.846 | 1.834 | 20.408 |
| ATOM | 1693 | C | ILE | B | 85 | 12.596 | 1.254 | 21.085 |
| ATOM | 1694 | O | ILE | B | 85 | 11.536 | 1.903 | 21.267 |
| ATOM | 1695 | CB | ILE | B | 85 | 14.308 | 3.115 | 21.137 |
| ATOM | 1696 | CG1 | ILE | B | 85 | 15.447 | 3.826 | 20.395 |
| ATOM | 1697 | CG2 | ILE | B | 85 | 14.673 | 2.840 | 22.589 |
| ATOM | 1698 | CD1 | ILE | B | 85 | 16.730 | 3.053 | 20.263 |
| ATOM | 1699 | N | GLY | B | 86 | 12.617 | -0.052 | 21.422 |
| ATOM | 1700 | H | GLY | B | 86 | 13.439 | -0.595 | 21.251 |
| ATOM | 1701 | CA | GLY | B | 86 | 11.481 | -0.702 | 22.028 |
| ATOM | 1702 | C | GLY | B | 86 | 11.557 | -0.748 | 23.538 |
| ATOM | 1703 | O | GLY | B | 86 | 12.412 | -0.165 | 24.238 |
| ATOM | 1704 | N | ARG | B | 87 | 10.614 | -1.489 | 24.149 |
| ATOM | 1705 | H | ARG | B | 87 | 10.012 | -2.072 | 23.604 |
| ATOM | 1706 | CA | ARG | B | 87 | 10.442 | -1.468 | 25.584 |
| ATOM | 1707 | C | ARG | B | 87 | 11.627 | -2.021 | 26.326 |
| ATOM | 1708 | O | ARG | B | 87 | 11.911 | -1.666 | 27.495 |
| ATOM | 1709 | CB | ARG | B | 87 | 9.200 | -2.271 | 25.949 |
| ATOM | 1710 | CG | ARG | B | 87 | 7.951 | -1.960 | 25.161 |
| ATOM | 1711 | CD | ARG | B | 87 | 6.956 | -3.074 | 25.219 |
| ATOM | 1712 | NE | ARG | B | 87 | 5.906 | -2.933 | 24.205 |
| ATOM | 1713 | HE | ARG | B | 87 | 5.790 | -2.039 | 23.772 |
| ATOM | 1714 | CZ | ARG | B | 87 | 5.119 | -3.953 | 23.856 |
| ATOM | 1715 | NH1 | ARG | B | 87 | 5.252 | -5.161 | 24.396 |
| ATOM | 1716 | 2HH1 | ARG | B | 87 | 5.958 | -5.326 | 25.085 |
| ATOM | 1717 | 1HH1 | ARG | B | 87 | 4.646 | -5.905 | 24.113 |
| ATOM | 1718 | NH2 | ARG | B | 87 | 4.180 | -3.751 | 22.939 |
| ATOM | 1719 | 1HH2 | ARG | B | 87 | 3.580 | -4.502 | 22.664 |
| ATOM | 1720 | 2HH2 | ARG | B | 87 | 4.073 | -2.848 | 22.524 |
| ATOM | 1721 | N | ASN | B | 88 | 12.413 | -2.937 | 25.731 |
| ATOM | 1722 | H | ASN | B | 88 | 12.206 | -3.237 | 24.800 |
| ATOM | 1723 | CA | ASN | B | 88 | 13.582 | -3.519 | 26.415 |
| ATOM | 1724 | C | ASN | B | 88 | 14.532 | -2.429 | 26.821 |
| ATOM | 1725 | O | ASN | B | 88 | 15.214 | -2.516 | 27.863 |
| ATOM | 1726 | CB | ASN | B | 88 | 14.285 | -4.605 | 25.559 |
| ATOM | 1727 | CG | ASN | B | 88 | 15.063 | -4.031 | 24.358 |
| ATOM | 1728 | OD1 | ASN | B | 88 | 14.515 | -3.245 | 23.612 |
| ATOM | 1729 | ND2 | ASN | B | 88 | 16.333 | -4.445 | 24.180 |
| ATOM | 1730 | 2HD2 | ASN | B | 88 | 16.875 | -4.099 | 23.414 |
| ATOM | 1731 | 1HD2 | ASN | B | 88 | 16.744 | -5.102 | 24.812 |
| ATOM | 1732 | N | LEU | B | 89 | 14.695 | -1.328 | 26.061 |
| ATOM | 1733 | H | LEU | B | 89 | 14.192 | -1.240 | 25.201 |
| ATOM | 1734 | CA | LEU | B | 89 | 15.597 | -0.234 | 26.452 |

FIG. 1 lee

```
ATOM   1735  C    LEU B  89      14.797   0.937  27.053
ATOM   1736  O    LEU B  89      15.293   1.734  27.879
ATOM   1737  CB   LEU B  89      16.421   0.232  25.236
ATOM   1738  CG   LEU B  89      17.400  -0.754  24.567
ATOM   1739  CD1  LEU B  89      18.215   0.002  23.573
ATOM   1740  CD2  LEU B  89      18.352  -1.458  25.570
ATOM   1741  N    LEU B  90      13.511   1.114  26.705
ATOM   1742  H    LEU B  90      13.082   0.486  26.056
ATOM   1743  CA   LEU B  90      12.698   2.221  27.257
ATOM   1744  C    LEU B  90      12.537   2.060  28.751
ATOM   1745  O    LEU B  90      12.575   3.033  29.533
ATOM   1746  CB   LEU B  90      11.311   2.258  26.628
ATOM   1747  CG   LEU B  90      11.232   2.730  25.168
ATOM   1748  CD1  LEU B  90       9.808   2.744  24.642
ATOM   1749  CD2  LEU B  90      11.831   4.105  24.982
ATOM   1750  N    THR B  91      12.315   0.843  29.271
ATOM   1751  H    THR B  91      12.218   0.055  28.663
ATOM   1752  CA   THR B  91      12.210   0.634  30.699
ATOM   1753  C    THR B  91      13.537   1.028  31.375
ATOM   1754  O    THR B  91      13.575   1.525  32.518
ATOM   1755  CB   THR B  91      11.893  -0.843  31.028
ATOM   1756  OG1  THR B  91      12.919  -1.676  30.504
ATOM   1757  HG1  THR B  91      12.722  -2.634  30.713
ATOM   1758  CG2  THR B  91      10.599  -1.285  30.418
ATOM   1759  N    GLN B  92      14.705   0.852  30.732
ATOM   1760  H    GLN B  92      14.707   0.497  29.797
ATOM   1761  CA   GLN B  92      15.920   1.190  31.433
ATOM   1762  C    GLN B  92      16.088   2.660  31.633
ATOM   1763  O    GLN B  92      16.807   3.137  32.527
ATOM   1764  CB   GLN B  92      17.127   0.680  30.682
ATOM   1765  CG   GLN B  92      17.076  -0.805  30.517
ATOM   1766  CD   GLN B  92      18.336  -1.314  29.900
ATOM   1767  OE1  GLN B  92      19.394  -0.720  30.059
ATOM   1768  NE2  GLN B  92      18.221  -2.411  29.195
ATOM   1769 1HE2  GLN B  92      19.022  -2.813  28.751
ATOM   1770 2HE2  GLN B  92      17.331  -2.856  29.095
ATOM   1771  N    ILE B  93      15.538   3.512  30.746
ATOM   1772  H    ILE B  93      15.016   3.153  29.972
ATOM   1773  CA   ILE B  93      15.693   4.937  30.899
ATOM   1774  C    ILE B  93      14.522   5.549  31.698
ATOM   1775  O    ILE B  93      14.438   6.773  31.940
ATOM   1776  CB   ILE B  93      15.981   5.657  29.548
ATOM   1777  CG1  ILE B  93      14.746   5.718  28.619
ATOM   1778  CG2  ILE B  93      17.223   5.060  28.874
ATOM   1779  CD1  ILE B  93      14.946   6.734  27.488
ATOM   1780  N    GLY B  94      13.617   4.731  32.263
ATOM   1781  H    GLY B  94      13.639   3.752  32.060
ATOM   1782  CA   GLY B  94      12.594   5.224  33.170
ATOM   1783  C    GLY B  94      11.443   5.846  32.432
ATOM   1784  O    GLY B  94      10.766   6.803  32.878
ATOM   1785  N    CYS B  95      11.134   5.354  31.225
ATOM   1786  H    CYS B  95      11.603   4.538  30.888
ATOM   1787  CA   CYS B  95      10.134   5.969  30.381
ATOM   1788  C    CYS B  95       8.750   5.512  30.764
ATOM   1789  O    CYS B  95       8.478   4.309  31.006
ATOM   1790  CB   CYS B  95      10.456   5.643  28.922
```

FIG. 1Iff

```
ATOM   1791  SG  CYS B  95       9.426   6.512  27.764
ATOM   1792  N   THR B  96       7.778   6.444  30.764
ATOM   1793  H   THR B  96       8.014   7.401  30.539
ATOM   1794  CA  THR B  96       6.379   6.163  31.108
ATOM   1795  C   THR B  96       5.390   6.970  30.254
ATOM   1796  O   THR B  96       5.567   8.171  30.066
ATOM   1797  CB  THR B  96       6.111   6.439  32.604
ATOM   1798  OG1 THR B  96       6.341   7.794  32.938
ATOM   1799  HG1 THR B  96       6.111   7.924  33.861
ATOM   1800  CG2 THR B  96       6.938   5.566  33.554
ATOM   1801  N   LEU B  97       4.302   6.321  29.809
ATOM   1802  H   LEU B  97       4.216   5.332  29.997
ATOM   1803  CA  LEU B  97       3.127   6.986  29.238
ATOM   1804  C   LEU B  97       2.336   7.681  30.358
ATOM   1805  O   LEU B  97       2.350   7.221  31.499
ATOM   1806  CB  LEU B  97       2.226   5.958  28.532
ATOM   1807  CG  LEU B  97       2.860   5.279  27.300
ATOM   1808  CD1 LEU B  97       2.101   3.986  26.957
ATOM   1809  CD2 LEU B  97       2.842   6.216  26.085
ATOM   1810  N   ASN B  98       1.637   8.777  30.024
ATOM   1811  H   ASN B  98       1.662   9.086  29.063
ATOM   1812  CA  ASN B  98       0.906   9.631  30.960
ATOM   1813  C   ASN B  98      -0.251  10.321  30.231
ATOM   1814  O   ASN B  98      -0.032  11.303  29.522
ATOM   1815  CB  ASN B  98       1.845  10.678  31.587
ATOM   1816  CG  ASN B  98       2.783  10.077  32.634
ATOM   1817  OD1 ASN B  98       3.926   9.739  32.335
ATOM   1818  ND2 ASN B  98       2.297   9.942  33.870
ATOM   1819 2HD2 ASN B  98       2.877   9.551  34.599
ATOM   1820 1HD2 ASN B  98       1.351  10.229  34.074
ATOM   1821  N   LEU B  99      -1.476   9.808  30.426
ATOM   1822  H   LEU B  99      -1.568   9.010  31.037
ATOM   1823  CA  LEU B  99      -2.709  10.288  29.797
ATOM   1824  C   LEU B  99      -3.816  10.589  30.815
ATOM   1825  O   LEU B  99      -3.630  10.272  32.011
ATOM   1826  CB  LEU B  99      -3.146   9.340  28.657
ATOM   1827  CG  LEU B  99      -3.714   7.932  28.941
ATOM   1828  CD1 LEU B  99      -2.767   7.057  29.774
ATOM   1829  CD2 LEU B  99      -5.134   7.943  29.528
ATOM   1830  OXT LEU B  99      -4.842  11.156  30.376
TER
```

FIG. 1 lgg

Database filename: hivpr.mdb
Number of structures: 10591
Tolerance (%) >= 1.05

| ResNum | TotOcc | TotFreq | Dist | WtAA | NumMut | MutList | NumList |
|---|---|---|---|---|---|---|---|
| 1 | 11 | 0 | 15.4 | P | 0 | | |
| 2 | 32 | 0 | 14.5 | Q | 0 | | |
| 3 | 38 | 0 | 12.1 | I | 0 | | |
| 4 | 106 | 0 | 13.0 | T | 0 | | |
| 5 | 100 | 0 | 11.3 | L | 0 | | |
| 6 | 47 | 0 | 14.3 | W | 0 | | |
| 7 | 58 | 0 | 12.8 | Q | 0 | | |
| 8 | 27 | 0 | 9.6 | R | 0 | | |
| 9 | 11 | 0 | 7.9 | P | 0 | | |
| 10 | 4004 | 37.8 | 9.2 | L | 3 | IVF | 3162 441 278 |
| 11 | 82 | 0 | 10.9 | V | 0 | | |
| 12 | 1117 | 10.5 | 13.7 | T | 5 | SEPAN | 241 185 158 155 117 |
| 13 | 1745 | 16.5 | 13.7 | I | 1 | V | 1717 |
| 14 | 646 | 6.1 | 17.0 | K | 1 | R | 623 |
| 15 | 1760 | 16.6 | 17.5 | I | 1 | V | 1709 |
| 16 | 361 | 3.4 | 20.9 | G | 1 | E | 254 |
| 17 | 56 | 0 | 22.4 | G | 0 | | |
| 18 | 242 | 2.3 | 20.5 | Q | 0 | | |
| 19 | 1340 | 12.7 | 18.3 | L | 4 | IVQT | 873 162 130 128 |
| 20 | 1549 | 14.6 | 15.4 | K | 4 | IRTM | 576 560 209 145 |
| 21 | 43 | 0 | 12.7 | E | 0 | | |
| 22 | 46 | 0 | 9.0 | A | 0 | | |
| 23 | 89 | 0 | 5.8 | L | 0 | | |
| 24 | 402 | 3.8 | 3.8 | L | 1 | I | 377 |

FIG. 8A

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 25 | 28 | 0 | 0.0 | D | 0 | | |
| 26 | 14 | 0 | 3.8 | T | 0 | | |
| 27 | 9 | 0 | 5.5 | G | 0 | | |
| 28 | 16 | 0 | 5.8 | A | 0 | | |
| 29 | 34 | 0 | 8.7 | D | 0 | | |
| 30 | 770 | 7.3 | 9.2 | D | 1 | N | 725 |
| 31 | 15 | 0 | 8.9 | T | 0 | | |
| 32 | 238 | 2.2 | 10.5 | V | 1 | I | 221 |
| 33 | 578 | 5.5 | 12.4 | L | 3 | VIF | 207 189 172 |
| 34 | 88 | 0 | 15.1 | E | 0 | | |
| 35 | 2790 | 26.3 | 18.6 | E | 1 | D | 2646 |
| 36 | 2780 | 26.2 | 20.2 | M | 2 | IV | 2549 129 |
| 37 | 3252 | 30.7 | 22.8 | N | 4 | DSET | 1253 1129 246 209 |
| 38 | 54 | 0 | 22.0 | L | 0 | | |
| 39 | 302 | 2.9 | 24.9 | P | 1 | S | 133 |
| 40 | 19 | 0 | 25.5 | G | 0 | | |
| 41 | 2249 | 21.2 | 26.0 | R | 1 | K | 2235 |
| 42 | 21 | 0 | 23.5 | W | 0 | | |
| 43 | 372 | 3.5 | 23.7 | K | 2 | TR | 166 144 |
| 44 | 12 | 0 | 22.6 | P | 0 | | |
| 45 | 208 | 2 | 20.0 | K | 1 | R | 170 |
| 46 | 2165 | 20.4 | 18.8 | M | 2 | IL | 1580 560 |
| 47 | 47 | 0 | 15.4 | I | 0 | | |
| 48 | 445 | 4.2 | 14.9 | G | 1 | V | 385 |
| 49 | 17 | 0 | 12.9 | G | 0 | | |
| 50 | 31 | 0 | 14.5 | I | 0 | | |
| 51 | 24 | 0 | 17.6 | G | 0 | | |
| 52 | 12 | 0 | 18.3 | G | 0 | | |
| 53 | 408 | 3.9 | 18.1 | F | 1 | L | 360 |

FIG. 8B

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 54 | 1661 | 15.7 | 18.0 | I | 1 | V | 1460 |
| 55 | 164 | 1.5 | 19.7 | K | 1 | R | 149 |
| 56 | 13 | 0 | 18.1 | V | 0 | | |
| 57 | 1194 | 11.3 | 19.7 | R | 1 | K | 1162 |
| 58 | 341 | 3.2 | 18.6 | Q | 1 | E | 317 |
| 59 | 20 | 0 | 19.4 | Y | 0 | | |
| 60 | 992 | 9.4 | 19.6 | D | 1 | E | 938 |
| 61 | 468 | 4.4 | 19.9 | Q | 1 | E | 285 |
| 62 | 2711 | 25.6 | 18.6 | I | 1 | V | 2685 |
| 63 | 8864 | 83.7 | 18.5 | L | 6 | PASTQH | 7245 380 321 266 226 162 |
| 64 | 2238 | 21.1 | 15.8 | I | 2 | VL | 1931 223 |
| 65 | 222 | 2.1 | 15.6 | E | 1 | D | 206 |
| 66 | 194 | 1.8 | 12.8 | I | 0 | | |
| 67 | 309 | 2.9 | 14.6 | C | 1 | S | 143 |
| 68 | 51 | 0 | 17.5 | G | 0 | | |
| 69 | 773 | 7.3 | 16.1 | H | 2 | QY | 376 206 |
| 70 | 478 | 4.5 | 17.0 | K | 1 | R | 359 |
| 71 | 3664 | 34.6 | 15.3 | A | 3 | VTI | 2301 1145 190 |
| 72 | 1494 | 14.1 | 17.2 | I | 3 | VTL | 650 409 126 |
| 73 | 1246 | 11.8 | 15.8 | G | 2 | ST | 932 185 |
| 74 | 658 | 6.2 | 15.4 | T | 2 | SA | 433 126 |
| 75 | 73 | 0 | 14.1 | V | 0 | | |
| 76 | 59 | 0 | 14.6 | L | 0 | | |
| 77 | 3533 | 33.4 | 16.1 | V | 1 | I | 3513 |
| 78 | 8 | 0 | 16.9 | G | 0 | | |
| 79 | 95 | 0 | 17.2 | P | 0 | | |
| 80 | 6 | 0 | 13.6 | T | 0 | | |
| 81 | 7 | 0 | 13.7 | P | 0 | | |
| 82 | 2208 | 20.8 | 11.0 | V | 2 | AT | 1668 284 |

FIG. 8C

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 83 | 44 | 0 | 9.7 | N | 0 | | |
| 84 | 1091 | 10.3 | 6.3 | I | 1 | V | 1073 |
| 85 | 213 | 2 | 5.7 | I | 1 | V | 198 |
| 86 | 16 | 0 | 5.3 | G | 0 | | |
| 87 | 32 | 0 | 7.3 | R | 0 | | |
| 88 | 706 | 6.7 | 10.4 | N | 2 | DS | 543 128 |
| 89 | 240 | 2.3 | 10.1 | L | 1 | M | 143 |
| 90 | 3429 | 32.4 | 8.3 | L | 1 | M | 3397 |
| 91 | 28 | 0 | 11.4 | T | 0 | | |
| 92 | 227 | 2.1 | 13.6 | Q | 1 | K | 169 |
| 93 | 3095 | 29.5 | 13.1 | I | 1 | L | 3041 |
| 94 | 15 | 0 | 13.6 | G | 0 | | |
| 95 | 100 | 0 | 10.6 | C | 0 | | |
| 96 | 6 | 0 | 11.2 | T | 0 | | |
| 97 | 83 | 0 | 10.7 | L | 0 | | |
| 98 | 44 | 0 | 14.2 | N | 0 | | |
| 99 | 35 | 0 | 16.4 | F | 0 | | |

FIG. 8D

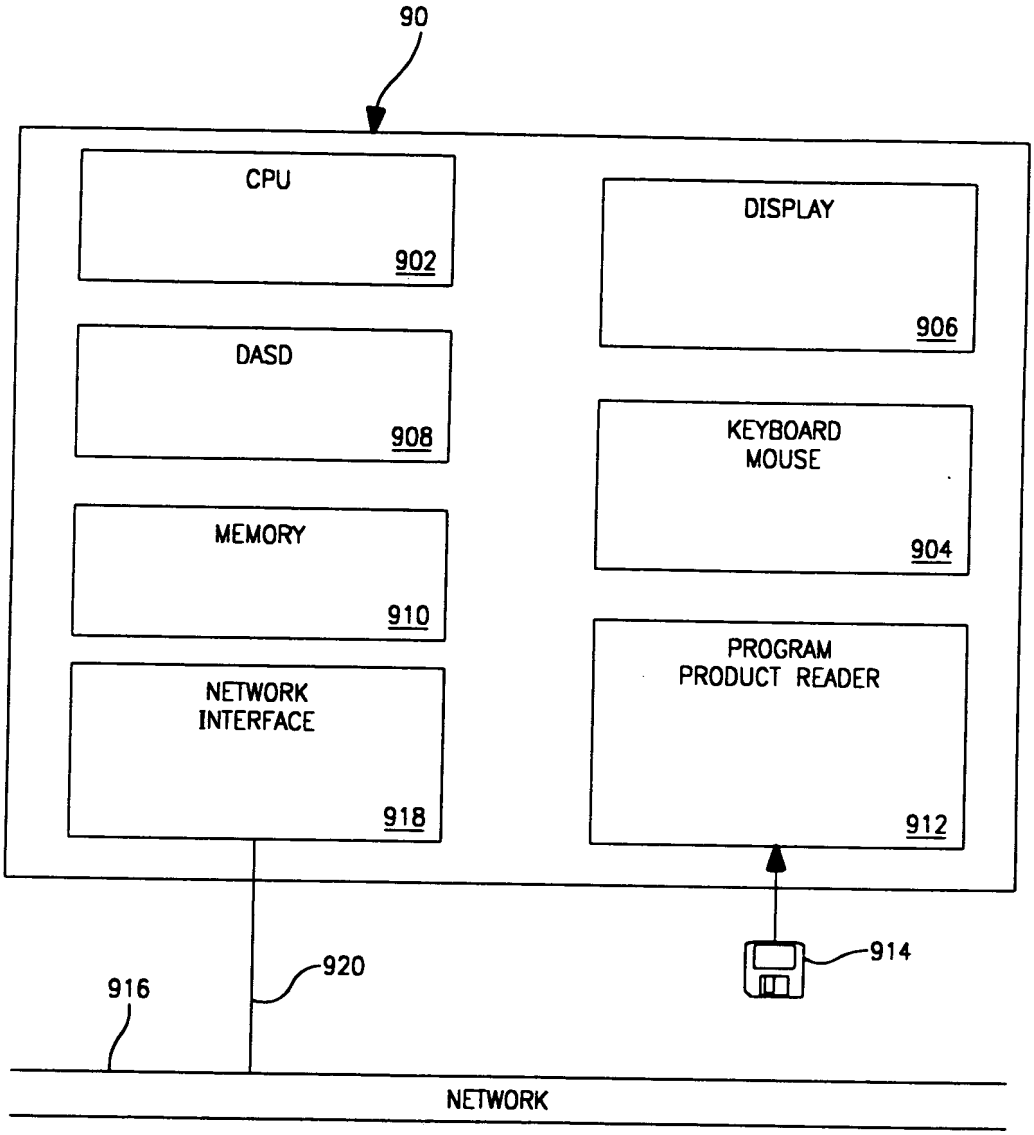



FIG. 9

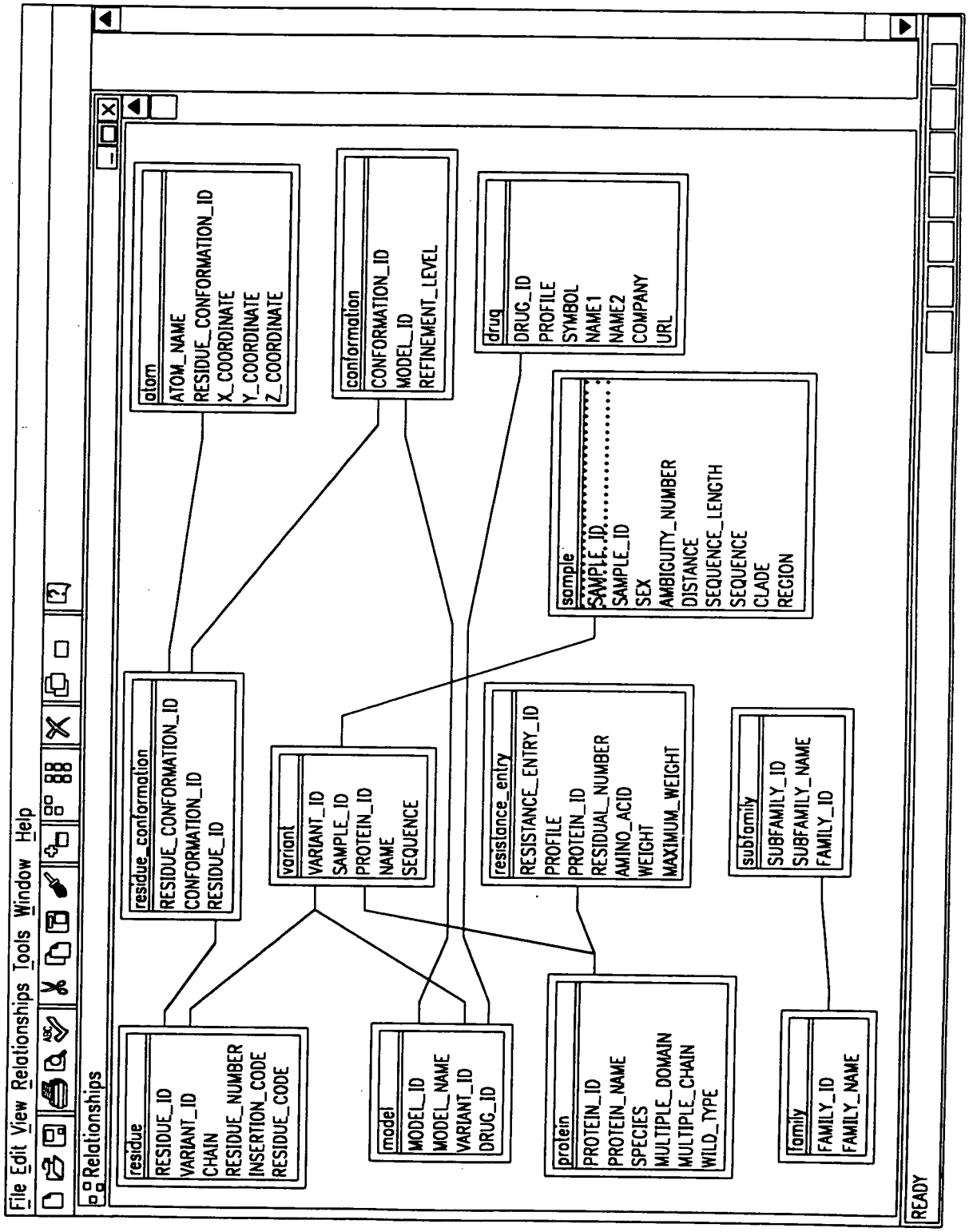



FIG. 10